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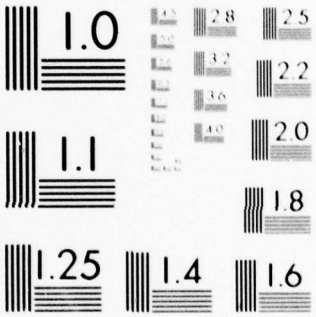

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The unsteady one-dimensional interaction of a planar flame, propagating through a fuel-lean premixture, with a parallel impervious noncatalytic wall is modeled as a Stefan-type problem incorporating one-step chemistry. Quantitative details concerning retardation of flame speed near an isothermal wall (pertinent to current cooled engines), and concerning acceleration of flame speed near an adiabatic wall (pertinent to proposed engines), are obtained. The time history of unburned hydrocarbon content varies with dimensionless Arrhenius activation energy, the order of the reaction chemistry, and the Lewis-Semenov number. Both temporally varying pressure, and also nonuniform fuel stratification, are discussed.

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ONE NEAR-TERM RESPONSE to current constraints of fuel cost, emissions standards, and acceptable performance is near-lean-limit operation of conventional engines. However, the reduced pressure and temperature achieved in homogeneous-charge four-stroke spark-ignition engines under such fuel-lean operation may lead to enhanced emission of partially oxidated, or pyrolyzed but unburned, hydrocarbons known to be toxic and/or carcinogenic [1].* Proper design of the number, location, timing, and energy of spark-ignition sources should preclude bulk-gas flame-out as a source of such emissions. However, the quench layers formed on cold cylinder surfaces (head wall, side wall, and piston crown) [2] are thickened under off-stoichiometric operation [3]; unless the cold unburned-hydrocarbon content of these quench layers can be oxidated by mixing with hot oxygen-rich bulk-gas products before being exhausted, the lean-operation strategy may be flawed. What seems required are experimental and theoretical investigations of the formation and fate of unburned hydrocarbons in reciprocating-piston-type internal combustion engines [4], to furnish as much engineering information as possible for the new designer who faces decisions concerning the relative merits of alternative engine modifications. This paper is one in a series in which the authors seek to contribute to this need.

The scope of the pertinent investigation should be broadened in view of recent interest in low-heat-transfer zircomium-oxide-sprayed engine components, and in adiabatic components of glass ceramics (such as silicon nitride and silicon carbide), particularly for larger engines [5,6]. If durable materials can be developed, not only are problems associated with the size and weight and reliability and maintenance of the cooling system reduced or even eliminated, but also currently wasted heat can

*Numbers in brackets designate references given at the end of the paper.

ABSTRACT

The unsteady one-dimensional interaction of a planar flame, propagating through a fuel-lean premixture, with a parallel impervious noncatalytic wall is modeled as a Stefan-type problem incorporating one-step chemistry. Quantitative details concerning retardation of flame speed near an isothermal wall (pertinent to current cooled engines), and concerning acceleration of flame speed near an adiabatic wall (pertinent to proposed engines), are obtained. The time history of unburned hydrocarbon content varies with dimensionless Arrhenius activation energy, the order of the reaction chemistry, and the Lewis-Semenov number. Both temporally varying pressure, and also nonuniform fuel stratification, are discussed.

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be utilized via engine compounding (if the exhaust port of the primary engine can survive hotter operating conditions).

Thus, interest centers on interaction of flames propagating through confined fuel-lean premixtures with (1) isothermal (cold) walls, and (2) adiabatic walls. Burning is anticipated to be retarded near cold walls and accelerated near adiabatic walls, but quantitative insight relating results to controllable parameters is extremely limited in the existing literature.

It seems premature to undertake the turbulent case when results for the laminar case are not yet available. Further, formulation for turbulent reacting flow in an automotive context is today highly conjectural [7], and turbulent fluctuations may be significantly reduced in the near-wall phenomena of interest. In any case, interest here is centered on laminar flow, though unsteady and nonisobaric conditions are ultimately to be included.

Though intermediate orientations can and do arise in practice, it is convenient to confine attention to two arrangements [8,9]: one in which the bulk-gas isotherms are parallel to the containing wall (henceforth termed the end-wall geometry) [10-14], and one in which the bulk-gas isotherms are perpendicular to the containing wall (henceforth termed the side-wall geometry) [15,16]. Elsewhere the authors intend to present both theoretical and experimental results for the side-wall geometry. It appears appropriate to confine the present discussions to theoretical results for the end-wall geometry only.

In general, attention is confined to unsteady one-dimensional flow in which a well-developed flame initially is propagating through a fuel-lean premixture; both the nonconfined (isobaric) and confined (nonisobaric) cases are of interest. How the properties of the flame become modified as a wall is approached is the central issue. Nevertheless, as a prerequisite, some properties of flame propagation away from walls must be established to serve as the starting (and reference) conditions. The dynamics is not central, once it is noted that the pressure is spatially invariant, though not in general temporally invariant, for the highly subsonic phenomena of interest. What is central, in addition to overall conservation of mass, is conservation of species and of heat; this conservation consists of a balance of convection, diffusion, and chemical reaction.

A conventional set of self-consistent approximations, often alluded to (in toto) as the Shvab-Zeldovich formulation [17], is adopted; this formulation has been of great engineering value in the analysis of a wide variety of aerothermochemical phenomena. A mixture of ideal gases of comparable molecular weight is taken to be present, such that a universal binary diffusion coefficient suffices, and one (constant, order-unity) Lewis-Semenov number may be introduced to characterize the ratio of thermal diffusivity to mass-transfer coefficients. The thermal diffusivity is taken to be inversely proportional to the square of the density. A universal constant heat capacity suffices, and thermodiffusion, barodiffusion, radiative transfer, and mechanical dissipation of energy are negligible. Most notably, a direct one-step irreversible exothermic mechanism describes the chemical-reaction mechanism, with an Arrhenius form appropriate for the specific rate constant occurring in the law of mass action [3]. The fact is that the detailed rates and multistep mechanisms of the actual higher-hydrocarbon/air chemical reaction, particularly with heterogeneous complications posed by the presence of a wall [18], are not known; once this chemical-kinetic compromise is accepted as currently necessary, the other simplifications follow from the considerations of a consistent level of approximation.

Accordingly, aside from the role of chemical reaction, which introduces the complexity of transcendental nonlinearity into the pertinent initial/boundary-value problems, treatment of parabolic linear constant-coefficient equations only, familiar from the field of heat conduction, is required. However, for Arrhenius activation temperature large relative to burned-gas temperature, the role of chemical reaction is limited to a spatial domain small relative to the domain in which a chemically frozen balance of convection and diffusion is an adequate description [19-21]. Here, this small spatial domain is reduced to a mathematical interface [22], which is a Dirac-delta-function-type sink for reactants, and source for products and chemical heat release. The interface is then a premixed thin flame, analogous to the Burke-Schumann diffusion flame [23] long employed in aerothermochemical flows involving unpremixed reactants; however, the flame without structure in the premixed case, in general, retains chemical-kinetic parameters (such as the Arrhenius activation energy), while the thin diffusion flame retains no chemical-kinetic parameters. Only in the special case of an adiabatic flow at Lewis-Semenov number unity is the premixed flame without structure independent of chemical-kinetic parameters [13]. Nevertheless, adoption of a thin flame (at which temperature and mass fractions are continuous, but their derivatives are discontinuous) is a significant simplification, even for the premixed reacting flow, because an overall solution is obtained simply by appropriately joining local solutions to heat-conduction-type problems at interfaces (flames). In that the position, as well as the temperature, of the flames must be found in the course of solution, thin-flame modeling reduces intractable aerothermochemical problems to tractable Stefan problems [24,25]. Not only are the conventional analytic procedures for treating Stefan problems available, but the authors have introduced novel techniques

for the aerothermochemical applications of relevance here. Such modeling may prove useful in a wider range of premixed reacting flows than the particular flame/wall interactions of interest here.

FORMULATION

Consider the unsteady, one-dimensional, low-Mach-number flow of a reacting premixture, where the chemical reaction is a direct, one-step, irreversible one between oxidant O and fuel F that generates gaseous product P, namely:

$$\nu_O\, O + \nu_F\, F \rightarrow \nu_P\, P, \tag{1}$$

where ν_i is the stoichiometric coefficient of species i, i = O, F, P. In the Shvab-Zeldovich approximation, the appropriate dimensional equations of conservation of mass, conservation of species, conservation of energy, and of state, for such a flow, are:

$$\frac{\partial \rho^*}{\partial t^*} + \frac{\partial(\rho^* u^*)}{\partial x^*} = 0 \;:\; \frac{\partial \psi^*}{\partial x^*} = \rho^*,\; \frac{\partial \psi^*}{\partial t^*} = -\rho^* u^*; \tag{2}$$

$$\rho^*\left(\frac{\partial Y_i}{\partial t^*} + u^*\frac{\partial Y_i}{\partial x^*}\right) - \frac{\partial}{\partial x^*}\left(\rho^* D^*\frac{\partial Y_i}{\partial x^*}\right) = -w^*, \quad i = O,F; \tag{3}$$

$$\rho^*\left(\frac{\partial T^*}{\partial t^*} + u^*\frac{\partial T^*}{\partial x^*}\right) - \frac{\partial}{\partial x^*}\left((\lambda^*/c_p^*)\frac{\partial T^*}{\partial x^*}\right) = (Q^*/c_p^*)w^* + (1/c_p^*)\frac{dp^*}{dt^*}\;; \tag{4}$$

$$p^* = \rho^* R^* T^*. \tag{5}$$

Here, t^* and x^* are the time and Cartesian spatial coordinates, respectively; u^* is the gas speed and ψ^* is the streamfunction; ρ^* and T^* are the density and temperature; R^* is the gas constant for the mixture, taken to be composed of species of comparable molecular weight; p^* is the pressure, taken to be a function of time only, from consideration of the equation of conservation of momentum; Y_i is the stoichiometrically-adjusted mass fraction of species i; D^* and λ^* are the mass-transfer and thermal-conductivity coefficients, respectively, and c_p^* is the (constant universal) heat capacity at constant pressure; and Q^* is the specific heat of combustion; while w^* is the reaction rate. In what follows, it is taken that the Lewis-Semenov number is a constant of order unity, i.e.,

$$Le = \frac{(\lambda^*/c_p^*)}{(\rho^* D^*)} = \text{const.} \sim O(1). \tag{6}$$

Further it is compatible with the accuracy characteristic of the Shvab-Zeldovich approximation to adopt

$$\rho^{*2} D^* = \text{const.} \tag{7}$$

In this presentation, the law of mass action, under an Arrhenius specific rate constant, modified to overcome the so-called cold-boundary difficulty, is

$$w^* = B'^* T^{*\alpha} \rho^{*\nu_O+\nu_F} Y_F^{\nu_F} Y_O^{\nu_O} \exp\left\{-\Theta^*/(T^* - T_u^*)\right\}. \tag{8}$$

where B'^* is the (constant) frequency factor; Θ^* is the (constant) Arrhenius activation temperature; T_u^* is the cold-boundary (i.e., cold-premixture) temperature; and α characterizes the pre-exponential thermal dependence of the reaction rate. While, in general, there need be no association of this dependence and order of reaction, for convenience (and within the accuracy of previously adopted approximations), here it is taken that

$$\alpha = (\nu_O + \nu_F) - 1. \tag{9}$$

It is also convenient to introduce the von Mises transformation $(x^*,t^*) \rightarrow (\psi^*,t^*)$, where the streamfunction ψ^* is defined in Eq. 2. Under this transformation, the species and energy conservation equations, 3 and 4, become

$$\frac{\partial Y_i}{\partial t^*} - (\rho^{*2}D^*)\frac{\partial^2 Y_i}{\partial \psi^{*2}} = -B'^*(p^*/R^*)^{(\nu_O+\nu_F)-1} Y_F^{\nu_F} Y_O^{\nu_O} \exp\left\{-\Theta^*/(T^* - T_u^*)\right\}; \tag{10}$$

$$\frac{\partial T^*}{\partial t^*} - (\rho^{*2}D^*)\,Le\,\frac{\partial^2 T^*}{\partial \psi^{*2}} = (1/c_p^*)\frac{1}{\rho^*}\frac{dp^*}{dt^*}$$
$$+ (Q^*/c_p^*)\,B'^*(p^*/R^*)^{(\nu_O+\nu_F)-1} Y_F^{\nu_F} Y_O^{\nu_O} \exp\left\{-\Theta^*/(T^* - T_u^*)\right\}; \tag{11}$$

while the (complementary) mass conservation and mapping equations are given by

$$\frac{\partial u^*}{\partial \psi^*} = \frac{\partial}{\partial t^*}\left(\frac{1}{\rho^*}\right) \;;\; \frac{\partial x^*}{\partial \psi^*} = \frac{1}{\rho^*}. \tag{12a,b}$$

To develop a nondimensional formulation, let

$$t = \frac{t^*}{(D_u^*/u_u^{*2})},\; \psi = \frac{\psi^*}{(\rho_u^* D_u^*/u_u^*)}\;; \tag{13}$$

$$Y(\psi,t) = \frac{Y_F(\psi^*,t^*)}{Y_{Fu}} = \frac{(1-\phi)}{\phi}\left(\frac{Y_O(\psi^*,t^*)}{Y_{Ob}} - 1\right). \tag{14}$$

$$T(\psi,t) = \frac{T^*(\psi^*,t^*) - T_u^*}{T_b^* - T_u^*}\;; \tag{15}$$

$$\rho(\psi,t) = \frac{\rho^*(\psi^*,t^*)}{\rho_u^*}, \quad p(t) = \frac{p^*(t)}{p_u^*}, \quad u(\psi,t) = \frac{u^*(\psi^*,t)}{u_u^*},$$

$$x(\psi,t) = \frac{x^*(\psi^*,t^*)}{(D_u^*/u_u^*)}. \tag{16}$$

Here, the subscript u denotes unburned (or cold-premixture) conditions; while, the subscript b denotes burned conditions (in the absence of heat losses, i.e., under adiabatic conditions). More specifically, u_u^* is the so-called adiabatic flame speed. Also, $\phi = (Y_{Fu}/Y_{Ou})$ is the (so-called) equivalence ratio, which is less than unity for cases of interest here. In this development, it is taken that $Y_{Fb} = 0$, such that $Y_{Ob} = (Y_{Ou} - Y_{Fu}) = [(1 - \phi)/\phi]Y_{Fu}$, and that $T_b^* = [T_u^* + (Q^*/c_p^*)Y_{Fu}]$. Further, $p_u^* = \rho_u^* R^* T_u^*$.

Thus, the nondimensional species and energy equations can be written as

$$\frac{\partial Y}{\partial t} - \frac{\partial^2 Y}{\partial \psi^2} = -\Lambda\, p^{(\nu_O + \nu_F) - 1}\, Y^{\nu_F} \left(1 + \frac{\phi}{(1-\phi)} Y\right)^{\nu_O} \exp\left\{-\beta \frac{(1-T)}{T}\right\}, \tag{17}$$

$$\frac{\partial T}{\partial t} - Le \frac{\partial^2 T}{\partial \psi^2} = \Lambda\, p^{(\nu_O + \nu_F) - 1}\, Y^{\nu_F} \left(1 + \frac{\phi}{(1-\phi)} Y\right)^{\nu_O} \exp\left\{-\beta \frac{(1-T)}{T}\right\} + \frac{\gamma-1}{\gamma} \frac{(1 + KT)}{Kp} \frac{dp}{dt}, \tag{18}$$

where

$$K = \frac{(T_b^* - T_u^*)}{T_u^*} = \frac{(Q^*/c_p^*)Y_{Fu}}{T_u^*}, \quad \gamma = \left(\frac{c_p^*}{c_v^*}\right) = \left(\frac{c_p^*}{(c_p^* - R^*)}\right). \tag{19}$$

$$\beta = \frac{Q^*}{(T_b^* - T_u^*)}. \tag{20}$$

$$\Lambda = \left(\frac{\beta^{*} D_u^*}{u_u^{*2}}\right)\left(\frac{p_u^*}{R^*}\right)^{(\nu_O + \nu_F) - 1} \left(\frac{1-\phi}{\phi}\right)^{\nu_O} Y_{Fu}^{(\nu_F + \nu_O) - 1} \exp(-\beta). \tag{21}$$

The nondimensional state, continuity, and mapping equations can be written as

$$\rho = \frac{p}{1 + KT}, \quad \frac{\partial u}{\partial \psi} = \frac{\partial}{\partial t}\left(\frac{1}{\rho}\right) = \frac{\partial}{\partial t}\left(\frac{(1 + KT)}{p}\right), \quad \frac{\partial x}{\partial \psi} = \frac{1}{\rho} = \frac{(1 + KT)}{p}. \tag{22}$$

Typically, the nondimensional activation temperature, β, is much greater than unity [3]; this observation is central to the analysis to follow. The quantity Λ plays the role of an eigenvalue in steady flame propagation; again, it is steady adiabatic flame propagation into a quiescent premixture characterized by p_u^*, T_u^*, Y_{Fu}, and ϕ that yields u_u^*, taken as known for species O, F reacting to form product P. For steady adiabatic laminar flame propagation for large β, it is known [19-21] that (1) the flow field may be divided into a chemically frozen preheat domain, of scale (D_u^*/u_u^*), in which convective diffusion occurs, and a relatively thinner reactive domain, of scale $\beta^{-1}(D_u^*/u_u^*)$, in which chemical reaction and diffusion balance; (2) that (except for very-near-stoichiometric conditions, i.e., $\phi \to 1$),

$$1 + \frac{\phi}{1-\phi} Y \to 1 \tag{23}$$

in the reaction zone, the only region in which chemical processes play a significant role (so $Y_O \simeq Y_{O_u}$ for all ψ,t from Eq. 14); and (3) that {if $\Gamma(z)$ denotes the (complete) gamma function of z [26]}

$$\Lambda = \beta^{\nu_F + 1} [2\Gamma(\nu_F + 1)\, Le^{\nu_F + 1}]^{-1} [1 + O(\beta^{-1})] \tag{24}$$

for the fuel-lean case. Accordingly, for more complicated phenomena involving combustion in fuel-lean premixtures characterized by large β, it appears convenient and appropriate to reduce the narrow reaction zone to a mathematical interface at $\psi = \Psi(t)$, with $\Psi(t)$, the interface location, a quantity to be found in the course of solution. For continuity of the dependent variables themselves, it is required that

$$Y \to 0, \; T \to \bar{H} = \bar{H}(t) \text{ as } \psi \to \Psi(t), \text{ for } t \geq 0, \tag{25}$$

with $\bar{H}(t)$, the temperature at the flame, another quantity to be found in the course of solution. The flame is anticipated to be a Dirac-delta-function-type source [26] for chemical heat and sink for reactants, such that first (and higher) spatial derivatives of the dependent variables (aside from the pressure) are discontinuous. Hence, in the vicinity of $\Psi(t)$, the equations for conservation of fuel and energy are well approximated by

$$\frac{\partial^2 Y}{\partial \psi^2} \doteq \Lambda\, p^{(\nu_O + \nu_F) - 1}\, Y^{\nu_F} \exp\left\{-\beta \frac{1-T}{T}\right\}, \tag{26}$$

$$Le \frac{\partial^2 T}{\partial \psi^2} \doteq -\Lambda\, p^{(\nu_O + \nu_F) - 1}\, Y^{\nu_F} \exp\left\{-\beta \frac{1-T}{T}\right\}. \tag{27}$$

Hence, in the vicinity of $\Psi(t)$,

$$\frac{\partial^2}{\partial \psi^2}(Y + Le\, T) = 0 \Longrightarrow Le\left\{\frac{\partial T[\Psi^+(t),t]}{\partial \psi} - \frac{\partial T[\Psi^-(t),t]}{\partial \psi}\right\} = \frac{\partial Y[\Psi^-(t),t]}{\partial \psi}, \tag{28}$$

if the convention is henceforth adopted that $Y[\psi \geq \Psi(t),t] = 0$. It suffices for the calculation of the dependence of the jump in Y_ψ on β and $\bar{H}(t)$ (using Eq. 26) to take

$$T(\psi,t) = \bar{H}(t) - (1/Le)\, Y(\psi,t) + \cdots . \tag{29}$$

The discrepancy is of the order of $1/\beta$ and would be eliminated formally in a derivation using singular perturbation theory. Accordingly, for $\varepsilon \ll 1$,

$$\int_{\Psi(t)-\varepsilon}^{\Psi(t)+\varepsilon} \frac{\partial^2 Y}{\partial\psi^2}\frac{\partial Y}{\partial\psi}\, d\psi \doteq \Lambda\, p^{(\nu_O+\nu_F)-1} \int_{\Psi(t)-\varepsilon}^{\Psi(t)+\varepsilon} Y^{\nu_F} \exp\left\{-\beta\,\frac{1-T}{T}\right\}\frac{\partial Y}{\partial\psi}\, d\psi \,. \tag{30}$$

or, from Eq. 29,

$$\left\{\frac{\partial Y[\Psi^-(t),t]}{\partial\psi}\right\}^2 = 2\Lambda\, p^{(\nu_O+\nu_F)-1}\int_0^\infty Y^{\nu_F}\exp\left\{-\beta\,\frac{(1-\bar{H})+(Y/Le)}{\bar{H}-(Y/Le)}\right\} dY, \tag{31}$$

where the upper limit has been extended to infinity by use of Laplace-integral-type (i.e., steepest-descent) concepts [26]. Expansion of the argument of the exponential gives

$$\left\{\frac{\partial Y[\Psi^-(t),t]}{\partial\psi}\right\}^2 \doteq 2\Lambda\, p^{(\nu_O+\nu_F)-1}\exp\left\{-\beta\,\frac{1-\bar{H}}{\bar{H}}\right\}\int_0^\infty Y^{\nu_F}\exp\left\{-\beta\,\frac{Y}{Le\,\bar{H}^2}\right\} dY; \tag{32}$$

$$\frac{\partial Y[\Psi^-(t),t]}{\partial\psi} \doteq -p^{\left((\nu_O+\nu_F)-1\right)/2}\,\bar{H}^{\nu_F+1}\exp\left\{-\frac{\beta}{2}\,\frac{1-\bar{H}}{\bar{H}}\right\}. \tag{33}$$

by Eq. 24.

These results may be anticipated to hold for vigorous burning only, such that a narrow reaction zone may be adequately approximated by equivalent interfacial conditions. Nevertheless, the results should be of qualitative use for less vigorous burning, in which the reaction zone is diffuse. The interfacial results presented here by heuristic arugment may be obtained more formally by application of multiple-scaling techniques of modern asymptotic analysis; actually, Zeldovich and Spalding intuitively used equivalent methodology decades ago [17].

The resulting Stefan-type problem [24,25] may be summarized as follows for the domain $t \geq 0$, $\psi_L \leq \psi \leq \psi_R$. For $\Psi(t) < \psi < \psi_R$, i.e., downstream of the flame, the species and energy equations are (Fig. 1)

$$Y = 0, \tag{34}$$

$$\frac{\partial h}{\partial t} - Le\,\frac{\partial^2 h}{\partial\psi^2} = \frac{\gamma-1}{\gamma}\,\frac{1+K\,h}{K\,p}\,\frac{dp}{dt}\,; \tag{35}$$

while for $\psi_L < \psi < \Psi(t)$, i.e., upstream of the flame, the species and energy equations are

$$\frac{\partial Y}{\partial t} - \frac{\partial^2 Y}{\partial\psi^2} = 0, \tag{36}$$

$$\frac{\partial H}{\partial t} - Le\,\frac{\partial^2 H}{\partial\psi^2} = \frac{\gamma-1}{\gamma}\,\frac{1+KH}{Kp}\,\frac{dp}{dt}\,. \tag{37}$$

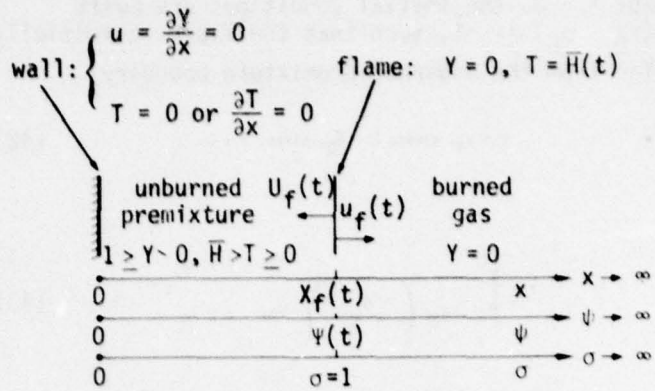

Fig. 1 - Schematic for a thin-flame, Stefan-type model of the unsteady one-dimensional isobaric flow in which a large-activation-energy laminar flame propagates toward an impervious noncatalytic wall, that is either isothermal (cold) or adiabatic. The purely diffusive-convective unburned-premixture region is characterized by finite fuel mass fraction Y and by temperature T below the temporally varying thin-flame temperature $\bar{H}(t)$; the purely diffusive-convective burned-gas region possesses no fuel. In the dimensionless Cartesian coordinate x, the flame site is denoted $X_f(t)$; in the von Mises (mass-weighted) coordinate, the corresponding variables are ψ, Ψ; in the Landau (flame-stabilized) coordinate, the corresponding variables are σ, 1. The gas speed at the flame is denoted u_f; the flame speed (in laboratory coordinates) is denoted U_f

The following notation has been introduced for convenience:

$$T(\psi,t) = \begin{cases} h(\psi,t) & \text{for} \quad \psi > \Psi(t) \\ H(\psi,t) & \text{for} \quad \psi < \Psi(t). \end{cases} \tag{38}$$

At the interface, i.e., for $\psi \to \Psi(t)$ $(t \geq 0)$, the boundary conditions for the dependent variables are

$$Y \to 0, \qquad h, H \to \bar{H}(t) \tag{39}$$

while the boundary conditions for the first derivatives of the dependent variables are

$$\left[\left(\frac{\partial Y}{\partial\psi} + Le\,\frac{\partial H}{\partial\psi}\right) - Le\,\frac{\partial h}{\partial\psi}\right]_\Psi \to 0 \tag{40}$$

with

$$\left(\frac{\partial Y}{\partial\psi}\right)_\Psi \to -p^{\left((\nu_O+\nu_F)-1\right)/2}\,\bar{H}^{\nu_F+1}\exp\left(-\frac{\beta}{2}\,\frac{(1-\bar{H})}{\bar{H}}\right). \tag{41}$$

For $t \to 0$, the initial conditions are [with $(\Psi_0 - \psi_L) >> 1$, such that the flame is initially far from the unburned-premixture boundary]

$$\Psi \to \Psi_0, \text{ given}; \ \bar{H} \to \bar{H}_0, \text{ given}; \ p \to 1. \tag{42}$$

$$Y \to \begin{cases} 0 & \text{for} \quad \psi \geq \Psi_0 \\ 1 - \exp\left(-\dfrac{(\Psi_0 - \psi)}{d_0}\right) & \text{for} \quad \psi \leq \Psi_0 \end{cases}; \tag{43}$$

$$H \to 1 - (1 - \bar{H}_0) \exp\left(-\frac{(\Psi_0 - \psi)}{Le\, b_0}\right), \ h \to 1 - (1 - \bar{H}_0) \exp\left(-\frac{(\psi - \Psi_0)}{Le\, c_0}\right), \tag{44}$$

where b_0, c_0, d_0 are given consts. close to unity in value, so the initial profiles are very similar to those occurring in laminar isobaric flame propagation. The right end-point boundary condition is

$$h \to 1 \text{ as } \psi \to \psi_R (t \geq 0); \tag{45}$$

while the left end-point boundary conditions are

$$H \to 0 \text{ or } \frac{\partial H}{\partial \psi} \to 0 \text{ as } \psi \to \psi_L (t \leq 0); \tag{46}$$

$$Y \to 1 \text{ or } \frac{\partial Y}{\partial \psi} \to 0 \text{ as } \psi \to \psi_L (t \leq 0). \tag{47}$$

For some cases to be considered below, the boundary and/or initial conditions given here are modified, but explicitness is preferred to generality for purposes of presentation. However, any initial conditions adopted are anticipated to be compatible with the boundary conditions to a high degree of accuracy. For brevity, the complementary relations (Eq. 22) are not repeated here, though it is noted that boundary conditions on the velocity at impervious walls are enforced, of course, in the obtaining of solutions.

One special case is deemed worthy of discussion at this point. For a semi-infinite domain (e.g., $\psi_R \to \infty$), the flow is well approximated as isobaric in many circumstances, such that $p(t) = 1$. If, in addition, the flow is adiabatic with Lewis-Semenov number $Le = 1$, then, under the provision that the following statements are compatible with the initial and boundary conditions of interest,

$$h = \bar{H} = 1 \text{ for } \psi \leq \Psi(t); \ Y + H = \bar{H} = 1 \text{ for } \psi \geq \Psi. \tag{48}$$

In this special circumstance,

$$\frac{\partial Y}{\partial \psi} \to -1 \Longrightarrow \frac{\partial H}{\partial \psi} \to 1 \text{ as } \psi \to \Psi^-. \tag{49}$$

independently of the chemical-kinetic parameter β. Because of this significant simplification, this special adiabatic case has been considered separately for the particular circumstance of a flame propagating isobarically toward an adiabatic, noncatalytic wall [13].

In the sense that the reaction order and Arrhenius activation temperature for a one-step pseudomechanism for the chemistry must be empirically assigned, the exponent on the pressure factor, the exponent on the pre-exponential temperature factor, and the nondimensional activation temperature in the exponential factor, all in the expression for the mass-fraction gradient at the flame, are available for assignment [3,27].

Solution to the Stefan-problem formulation may be sought by direct numerical integration; this can be a challenging task to accomplish. Thus, the procedure preferred here is to recast the problem in a form such that the two-independent-variable dependence is reduced to dependence on a single independent variable, time. This may be achieved by use of the method of weighted residuals, or, more simply, by use of a straightforward integral method [28]; the result is an initial-value problem, consisting of simultaneous quasilinear ordinary differential equations in time, with appropriate starting conditions. The adequacy of this approximate procedure depends upon the ability to anticipate the spatial variation of the dependent variables. An alternative method to reduction to a one-independent-variable problem is to introduce the integral transform over space, with the inversion leading to two simultaneous nonlinear Volterra integral equations [26] for $\bar{H}(t)$, $\Psi(t)$; while this reduction is formally exact for cases of interest, convergence of the iterative technique required for solution of the integral equations must be achieved.

For completeness, it may be remarked that the simplification of the Stefan-problem formulation is based on the smallness of the reaction-zone thickness relative to the preheat-zone thickness, for large dimensionless Arrhenius activation temperature. Phenomena in the burned-gas region are taken to occur on the diffusive scale of the preheat zone. Now, in fact, a third spatial scale implicit in the adoption of the range $|\psi_R - \psi_L|$ has been introduced; in the Cartesian coordinate, reference may be made to the dimension of the "container" L^*; if the Peclet number Pe based on adiabatic flame speed is large, i.e., if $Pe \equiv L^*/(D_u^*/u_u^*) >> 1$, then even the diffusive-convective preheat and post-flame domains become narrow relative to scale L^*. In this circumstance, the diffusive terms may be dropped from the Stefan-problem formulation, provided the effect of the flame is appropriately accounted for in the resulting nondiffusive problem. In such a nondiffusive formulation, the

dependent variables themselves (except for the pressure) are discontinuous across the parametrically-inserted flame. Further details on this level of approximation are deferred to later publications; here, results for the already-developed Stefan problem, retaining the diffusive scale, are obtained.

PROBLEMS IN FLAME PROPAGATION

TRANSIENTS - Before problems including flame/wall interaction are undertaken, some unsteady flame propagation problems in the infinite domain $-\infty \leq \psi \leq \infty$ are examined to elucidate the formulation, the methods of solution, and some properties of the phenomena under study. Here the integral method is used to study the effect of Lewis-Semenov number on reattainment of steady flame propagation after a small heat extraction from, or addition to, the flame.

The isobaric initial/boundary-value problem is given by Eqs. 34-44 and Eq. 22, with $p \equiv 1$, $\psi_L \to -\infty$, $\psi_R \to \infty$, $\psi_0 \equiv 0$. The boundary conditions (Eqs. 45-47) become

$$h \to 1 \text{ as } \psi \to \infty \text{ (for } t \geq 0); \; H \to 0, \; Y \to 1 \text{ as } \psi \to -\infty \text{ (for } t \geq 0). \tag{50}$$

In anticipation of an integral method of solution, results are sought in the forms, compatible with Eq. 39,

$$h = 1 - (1-\overline{H}) \exp\left\{-(\psi-\Psi)/Le\, c\right\} \quad \text{for} \quad \Psi \leq \psi < \infty, \; t \geq 0; \tag{51}$$

$$H = \overline{H} \exp\left\{-(\Psi-\psi)/Le\, b\right\}, \tag{52}$$

$$Y = 1 - \exp\left\{-(\Psi-\psi)/d\right\} \quad \text{for} \quad -\infty < \psi \leq \Psi, \; t \geq 0, \tag{53}$$

with c, b, d, as well as $\overline{H}$ and Ψ, = fncs(t). These forms are compatible with the initial conditions (Eqs. 42-44) if $c \to c_0$, $b \to b_0$, $d \to d_0$, and $\overline{H} \to \overline{H}_0$ as $t \to 0$. Insertion of Eqs. 51-53 in Eqs. 40-41 yields

$$\frac{1}{d} = \overline{H}^{\nu_F + 1} \exp\left\{-\frac{\beta}{2}\frac{1-\overline{H}}{\overline{H}}\right\}, \quad \frac{(1-\overline{H})}{c} = \frac{\overline{H}}{b} - \frac{1}{d}. \tag{54}$$

At t = 0, for given values of $\overline{H}_0$ and c_0, these relations give b_0 and d_0; for $\overline{H}(t) = 1$, c(t) is, in general, irrelevant. If $\overline{H}_0$ is close to unity, so are b_0 and d_0.

The evolution in time of the solutions (Eqs. 51-53) requires the finding of b(t), c(t), d(t), $\overline{H}(t)$, and $\Psi(t)$. Two algebraic eqquations are obtained by the substitution of Eqs. 51-53 in integrals of Eqs. 35-37. For example, if prime denotes ordinary derivative with respect to time, from Eq. 36

$$\int_{-\infty}^{\Psi} \frac{\partial Y}{\partial t}\, d\psi = \int_{-\infty}^{\Psi} \frac{\partial^2 Y}{\partial \psi^2}\, d\psi = \left(\frac{\partial Y}{\partial \psi}\right)_{\Psi} \Longrightarrow \tag{55a}$$

$$\int_{-\infty}^{\Psi} \left[\exp\left\{-\frac{(\Psi-\psi)}{d}\right\}\right]\left[\frac{1}{d^2}\left\{d\Psi' - (\Psi-\psi)d'\right\}\right] d\psi = -\frac{1}{d} \Longrightarrow \tag{55b}$$

$$d(\Psi' - d') = -1. \tag{55c}$$

Similarly, Eq. 35 gives

$$\overline{H}' - (1-\overline{H})\left[\frac{\Psi'}{Le\, c} + \frac{c'}{c}\right] = -\frac{(1-\overline{H})}{Le\, c^2}, \tag{56}$$

and Eq. 37 gives

$$Le\, b^2\left(\frac{\overline{H}'}{\overline{H}} - \frac{\Psi'}{Le\, b} + \frac{b'}{b}\right) = 1. \tag{57}$$

If Eq. 54 is enforced in algebraic form at t = 0 to determine b_0, d_0, then the partly differential set is conveniently rendered a set of coupled quasilinear ordinary differential equations by differentiation of Eq. 54:

$$\frac{d'}{d} + \left[(\nu_F + 1) + \frac{\beta}{2\overline{H}}\right]\frac{\overline{H}'}{\overline{H}} = 0, \tag{58}$$

$$\left(\frac{1}{b} + \frac{1}{c}\right)\overline{H}' + \frac{1}{d^2}d' - \frac{\overline{H}}{b^2}b' + \frac{1-\overline{H}}{c^2}c' = 0. \tag{59}$$

For $\overline{H}_0 = \overline{H} \equiv 1$, Eq. 56 is an identity, c plays no role, $d = d_0 \equiv 1$ from Eq. 54 and/or Eq. 58, $b = d \equiv 1$ from Eq. 54 and/or Eq. 58, and $\Psi' = -1$ from Eq. 55c and/or Eq. 57, so that $\Psi = -t$, since $\Psi_0 = 0$. Thus, as a special case, this set can recover steady laminar flame propagation (here expressed in a laboratory, as opposed to a flame-fixed, frame of reference). Since $\overline{H} \doteq 1$ for appreciable reaction, Eq. 58 gives interesting insight into the relative importance of the reaction order ν_F and the non-dimensional activation temperature β. Incrementing β by two has the same effect on the solution as incrementing ν_F by unity for $\overline{H} \doteq 1$; since $\beta = O(10)$, $\nu_F = O(1)$, typically, an appreciable change in ν_F, such as an increase from one to two, has modest effect on the results.

The following results concerning the effect of Lewis-Semenov number Le and of $\overline{H}_0$ on the rate of recovery of laminar propagation speed are obtained by numerical integration of Eqs. 55c, 56-59, for $c_0 = 1$, $\beta = 10$, $\nu_F = 1$. For Le = 1,

$\overline{H}_0 = 0.9$ (such that $\Psi_0' \doteq -0.25$) results in $\overline{H} \doteq 0.97$ and $\Psi' = 0.9$ for $t = 10$, but $\overline{H}_0 = 0.5$ (such that $\Psi_0' \doteq -0.005$) results in effectively no recovery at all, even by $t = 100$. Hence, for too large a perturbation, steady flame propagation effectively is not recovered, according to the model. Also, for Le = 1, $\overline{H}_0 = 0.99$ (such that $\Psi_0' \doteq -0.93$) results in $\Psi' = -0.99$ for $t \doteq 3$, but $\overline{H}_0 = 1.01$ (such that $\Psi_0' = -1.07$) results in $\Psi' = -1.01$ for $t \doteq 1.9$; hence, recovery is faster for flame-temperature augmentation than for flame-temperature depression. For $\overline{H}_0 = 0.9$, at Le = 0.7 (such that $\Psi_0' = -0.26$), $\overline{H} \doteq 0.99$ at $t \doteq 17.5$ and $\Psi' = -0.99$ at $t \doteq 23.5$; for $\overline{H}_0 = 0.9$, at Le = 1.3 (such that $\Psi_0' = -0.25$), $\overline{H} \doteq 0.99$ at $t \doteq 7.9$ and $\psi' = -0.99$ at $t \doteq 6.5$ Thus, for larger Lewis-Semenov number, both the flame temperature and the flame speed are recovered sooner. It should be noted that the influence of the Lewis-Semenov number on the adiabatic flame speed itself is implicit in the nondimensionalization; the influence of the Lewis-Semenov number on the rate of recovery of steady flame propagation after an initial temperature perturbation is the matter under study.

STRATIFICATION - Here, the Fourier integral transform is used to derive Volterra integral equations describing the effect of nonuniform stoichiometry of the premixture on laminar flame propagation; in particular, the error incurred by using locally an appropriate steady-laminar-flame-propagation formula to obtain the accelerating or decelerating flame speed is sought. Of course, nonuniform stoichiometry of the fuel/air premixture is of current automotive interest because of stratified-charge engines.

The initial/boundary-value problem posed by Eqs. 34-47, and Eq. 22, is recast to allow a more general initial condition, and to incorporate the conditions (Eqs. 40-41) in the partial differential equations (35-37). Thus, over the domain $-\infty \leq \psi \leq \infty$, $t \geq 0$,

$$\frac{\partial Y}{\partial t} - \frac{\partial^2 Y}{\partial \psi^2} = -F\,\delta(\psi - \Psi), \tag{60}$$

$$\frac{\partial T}{\partial t} - Le\,\frac{\partial^2 T}{\partial \psi^2} = F\,\delta(\psi - \Psi), \tag{61}$$

where $\delta(z)$ is the Dirac delta function, $\Psi(t)$ again denotes the position of the flame, and, by definition,

$$F = \overline{H}^{\nu F+1} \exp\left\{-\frac{\beta}{2}\,\frac{1-\overline{H}}{\overline{H}}\right\}, \tag{62}$$

where, again, $\overline{H} = \overline{H}(t)$ denotes the flame temperature.

As $t \to 0$,

$$\overline{H} \to \overline{H}_0 \equiv 1,\ \Psi \to \Psi_0 \equiv 0,\ \Psi' \to \Psi_0' \equiv -1; \tag{63}$$

$$Y \to \begin{cases} 1 - \exp(\psi) + A\,S(-\psi-L) & \text{for } \psi \leq 0 \quad (64a) \\ 0 & \text{for } \psi \geq 0, \quad (64b) \end{cases}$$

$$T \to \begin{cases} \exp(\psi/Le) & \text{for } \psi \leq 0, \\ 1 & \text{for } \psi \geq 0, \end{cases} \tag{65}$$

where $S(z)$ is the Heaviside unit step function. The step-type increment (or decrement) to the upstream unburned premixture is characterized by a magnitude A at distance L from the initial flame site in the streamfunction coordinate ψ. The larger L, the more the step function diffuses to a smoothed-out transition from $Y = 1$ to $Y = (1 + A)$ before the flame arrives.

The boundary conditions are

$$Y \to (1+A),\ T \to 0 \text{ as } \psi \to -\infty \text{ (for } t \geq 0);\ Y \to 0,\ T \to 1 \text{ as } \psi \to \infty \text{ (for } t \geq 0). \tag{66}$$

Clearly the flame propagates from its initial site at the origin in the direction of negative ψ.

The Fourier transform pair over the spatial coordinate is introduced:

$$\overline{Y}(s,t) = \int_{-\infty}^{\infty} Y(\psi,t)\exp(-s\psi)d\psi \Longleftrightarrow Y(\psi,t) = \frac{1}{2\pi i}\int_{-\infty}^{\infty} \overline{Y}(s,t)\exp(s\psi)ds, \tag{67}$$

with the transform parameter $s \equiv i\xi$. For brevity, only the mass-fraction equation is developed; the temperature equation is readily seen to be similarly treated, so only the result is stated.

If tentatively the function F is formally treated as known, and if contributions from the integrations by parts are ignored (because the contour of the inversion integral with respect to singularities on the real axis is to be so chosen that the boundary conditions are incorporated), then application of the transform gives

$$\frac{\partial \overline{Y}}{\partial t} - s^2\,\overline{Y} = -F\exp(-s\Psi); \tag{68}$$

standard introduction of an integrating factor for this first-order differential equation gives

$$\overline{Y}(s,t) = \overline{Y}(s,0)\exp(s^2 t) - \int_0^t F(t')\exp\left\{s^2(t-t') - s\Psi(t')\right\}dt'. \tag{69}$$

Further, the taking of the transform of the initial condition gives

$$\bar{Y}(s,0) = -\frac{1}{s} + \frac{1}{s-1} - \frac{A}{s}\exp(Ls). \tag{70}$$

Inversion of the contour integrals [29] gives

$$Y(\psi,t) = \frac{1}{2}\,\mathrm{erfc}\left(\frac{\psi}{2t^{1/2}}\right) - \frac{1}{2}\exp(t+\psi)\,\mathrm{erfc}\left(t^{1/2} + \frac{\psi}{2t^{1/2}}\right) + \frac{A}{2}\,\mathrm{erfc}\left(\frac{\psi+L}{2t^{1/2}}\right) - \frac{1}{2\pi^{1/2}}\int_0^t \frac{F(t')}{(t-t')^{1/2}}\exp\left\{-\frac{[\psi-\psi(t')]^2}{4(t-t')}\right\}dt'. \tag{71}$$

The physical role of each term is now noted. Each of the first three terms on the right-hand side of Eq. 71 gives the time evolution of one of the three terms on the right-hand side of the initial condition (Eq. 64a); the first term of Eq. 71 is derived from the first term of Eq. 64a, etc. The fourth term on the right-hand side of Eq. 71 is consumption at the thin flame.

The result of Eq. 71 is given in laboratory coordinates; it is convenient to transform to flame-fixed coordinates:

$$(\psi,t) \to (\zeta,t), \text{ with } \zeta = \psi + m(t). \tag{72}$$

Eq. 71 is rewritten:

$$Y(\zeta,\psi) = \frac{1}{2}\,\mathrm{erfc}\left(\frac{\zeta-m(t)}{2t^{1/2}}\right) - \frac{1}{2}\exp\left(\zeta+t-m(t)\right)\mathrm{erfc}\left(\frac{\zeta+2t-m(t)}{2t^{1/2}}\right) + \frac{A}{2}\,\mathrm{erfc}\left(\frac{\zeta-m(t)+L}{2t^{1/2}}\right) - \frac{1}{2\pi^{1/2}}\int_0^t \frac{F(t')}{(t-t')^{1/2}}\exp\left\{-\frac{[\zeta-m(t)+m(t')]^2}{4(t-t')}\right\}dt'. \tag{73}$$

The flame is situated at $\zeta = 0$ for all time t. *Enforcement of Eq. 39 gives*

$$0 = \frac{1}{2}\,\mathrm{erfc}\left(-\frac{m(t)}{2t^{1/2}}\right) - \frac{1}{2}\left\{\exp\left(t-m(t)\right)\right\}\left\{\mathrm{erfc}\left(\frac{2t-m(t)}{2t^{1/2}}\right)\right\} + \frac{A}{2}\,\mathrm{erfc}\left(\frac{L-m(t)}{2t^{1/2}}\right) - \frac{1}{2\pi^{1/2}}\int_0^t \frac{F(t')}{(t-t')^{1/2}}\exp\left\{-\frac{[m(t)-m(t')]^2}{4(t-t')}\right\}dt'. \tag{74}$$

For $A = 0$, $F = 1$, $m = t$ is a solution of this integral equation; for $A \neq 0$, $\bar{H} \neq 1$, so $F \neq 1$, and $\bar{H}$ and m must be found. Whereas Eq. 74 gives one equation for the two unknowns, the second is obtained from consideration of Eqs. 61, 62, 65 and 66. It is found that

$$h(\psi,t) = \frac{1}{2}\,\mathrm{erfc}\left(\frac{\zeta-m(t)}{2(\mathrm{Le}\ t)^{1/2}}\right) + \frac{1}{2}\exp\left[\frac{\zeta+t-m(t)}{\mathrm{Le}}\right]\mathrm{erfc}\left(\frac{\zeta+2t-m(t)}{2(\mathrm{Le}\ t)^{1/2}}\right) + \frac{1}{2(\pi\,\mathrm{Le})^{1/2}}\int_0^t \frac{F(t')}{(t-t')^{1/2}}\exp\left\{-\frac{[\zeta-m(t)+m(t')]^2}{4\,\mathrm{Le}(t-t')}\right\}dt'. \tag{75}$$

Enforcement of Eq. 39 gives, if it is recalled that $h(\psi,t) \to \bar{H}(t)$ as $\psi \to \Psi(t)$,

$$\bar{H}(t) = \frac{1}{2}\,\mathrm{erfc}\left(\frac{m(t)}{2(\mathrm{Le}\ t)^{1/2}}\right) + \frac{1}{2}\exp\left(\frac{t-m(t)}{\mathrm{Le}}\right)\mathrm{erfc}\left(\frac{2t-m(t)}{2(\mathrm{Le}\ t)^{1/2}}\right) + \frac{1}{2(\pi\,\mathrm{Le})^{1/2}}\int_0^t \frac{F(t')}{(t-t')^{1/2}}\exp\left\{-\frac{[m(t)-m(t')]^2}{4\,\mathrm{Le}(t-t')}\right\}dt'. \tag{76}$$

For $\bar{H} = 1$ so that $F = 1$, $m = t$ is a solution of this integral equation for all finite values of Le. Eqs. 74 and 76 constitute the coupled relations for $\bar{H}$ and m; once these two unknown functions of time are determined, substitution in Eqs. 73 and 75, or then-straightforward numerical integration of Eqs. 60-66, yields the mass-fraction and temperature profiles at any (ζ,t).

Because a convergent iterative procedure for the treatment of Eqs. 74 and 76 is not an entirely trivial matter, some discussion is given here, prior to presentation of numerically-obtained results. First, the integral term in Eq. 76, denoted $I_2[t,m(t);\mathrm{Le},\nu_F,\beta]$, and the integral term in Eq. 74, denoted $I_1[t,m(t);\mathrm{Le},\nu_F,\beta] = I_2[t,m(t);1,\nu_F,\beta]$ are integrated by use of linear interpolation, as now indicated. Discrete time intervals of interest are selected: t_s, $s = 1,2,3, \ldots$, where $t_{s+1} > t_s$ and $t_1 = 0$. Then, for example,

$$I_2[t_s,m(t_s);\mathrm{Le},\nu_F,\beta] = \frac{1}{2(\pi\,\mathrm{Le})^{1/2}}\sum_{j=1}^{s-1}\int_{t_j}^{t_{j+1}} \frac{Q_j[t_j',\bar{H}(t_j'),m(t_j');t_s,m(t_s);\mathrm{Le},\nu_F,\beta]}{(t_s-t_j')^{1/2}}\,dt_j', \tag{77}$$

where t_j' is a dummy variable of integration. Here

$$Q_j[t_j',\bar{H}(t_j'),m(t_j');t_s,m(t_s);\mathrm{Le},\nu_F,\beta] \equiv F[t_j',\bar{H}(t_j');\nu_F,\beta]\exp\left\{-\frac{[m(t_s)-m(t_j')]^2}{4\,\mathrm{Le}(t_s-t_j')}\right\}$$
$$\equiv \left(\bar{H}(t_j')\right)^{\nu_F+1}\exp\left\{-\frac{\beta}{2}\frac{\left(1-H(t_j')\right)}{\bar{H}(t_j')}\right\}\exp\left\{-\frac{[m(t_s)-m(t_j')]^2}{4\,\mathrm{Le}(t_s-t_j')}\right\}$$
$$\doteq Q_j[t_j,\bar{H}(t_j),m(t_j);t_s,m(t_s);\mathrm{Le},\nu_F,\beta] - \frac{Q_{j+1}[t_{j+1},\bar{H}(t_{j+1}),m(t_{j+1});\cdots] - Q_j[t_j,\cdots]}{t_{j+1}-t_j}\left[(t_j-t_s)+(t_s-t_j')\right] \tag{78}$$

over the domain $t_j \leq t_j' \leq t_{j+1}$. Substitution of Eq. 78 in Eq. 77 and integration give $I_2[t_s,m(t_s);\mathrm{Le},\nu_F,\beta]$ as an algebraic, as opposed to integral, expression. For Le = 1, Eqs. 74 and 76 sum to

$$\bar{H}(t_s) = 1 + \frac{A}{2}\,\mathrm{erfc}\left[\frac{L-m(t_s)}{2\,t_s^{1/2}}\right]; \tag{79}$$

Use of Eq. 79 in Eq. 76, together with the concepts of Eqs. 77 and 78, yields one transcendentally nonlinear algebraic equation for one unknown, $m(t_s)$. A first guess may be obtained by linear extrapolation from $m(t_{s-1})$ and $m(t_{s-2})$; for early times, $m(t) \doteq t$ furnishes guidance. A second guess may be obtained by perturbing the first guess by a small amount. Newton's rule, with finite difference approximation of the first derivative based on the last two iterates from $m(t_s)$, quickly yields effectively invariant succesive iterates for $m(t_s)$ -- and, by use of Eq. 79,

for $\overline{H}(t_s)$ -- and, hence, quickly achieves convergence to a solution for t_s. Now, let $s \to (s+1)$, i.e., increment time, and repeat the procedure. For Le $\neq$ 1, an analogue to Eq. 79 is obtained as follows: multiply Eq. 74 by $(\mathrm{Le})^{-1/2}$ and, then, subtract Eq. 76 from Eq. 74 to produce

$$\begin{aligned}\overline{H}(t_s) = {} & \frac{1}{2}\left\{\mathrm{erfc}\left(\frac{m(t_s)}{2(\mathrm{Le}\ t_s)^{1/2}}\right) - \frac{1}{(\mathrm{Le})^{1/2}}\,\mathrm{erf}\left(\frac{-m(t_s)}{2\ t_s^{1/2}}\right)\right\} \\ & + \frac{1}{2}\left\{\exp\left(\frac{t_s - m(t_s)}{\mathrm{Le}}\right)\mathrm{erfc}\left(\frac{2\ t_s - m(t_s)}{2(\mathrm{Le}\ t_s)^{1/2}}\right)\right. \\ & \left. - \frac{1}{(\mathrm{Le})^{1/2}}\exp\left(t_s - m(t_s)\right)\mathrm{erfc}\left(\frac{2\ t_s - m(t_s)}{2\ t_s^{1/2}}\right)\right\} \\ & + \left\{I_2[t_s, m(t_s); \mathrm{Le}, \nu_F, \beta] - \frac{1}{(\mathrm{Le})^{1/2}}\, I_2[t_s, m(t_s); 1, \nu_F, \beta]\right\}. \end{aligned} \tag{80}$$

The (small) difference of the last line of Eq. 80 is evaluated as a number, by use of the best current estimates for $m(t_s)$, $\overline{H}(t_s)$; the first three lines of Eq. 80 are left as written. Then Eq. 80, for Le $\neq$ 1, serves the analogous role that Eq. 79 serves for Le = 1, i.e., substitution of Eq. 80 in Eq. 76 gives one nonlinear algebraic equation for $m(t_s)$, to be solved by iteration (using Newton's rule to obtain the root) until invariance of successive iterates for $m(t_s)$ indicates convergence. Use of this result for $m(t_s)$ in the first three lines of Eq. 80 yields an updated $\overline{H}(t_s)$. These values for $m(t_s)$, $\overline{H}(t_s)$ become the most current estimates, and the entire procedure can be repeated until convergence is obtained.

Results are presented in Figs. 2 through 4; spatial profiles for Y and T, at fixed time t, may be more readily obtained from numerical integration of Eqs. 60-66, with $\overline{H}(t)$ and $\psi(t)$ known, than from Eqs. 73 and 75. A question arises concerning how adequate Eqs. 21 and 24 are as a means of obtaining the instantaneous flame speed when the flame is propagating through the stratification gradient, such that the effective upwind mass fraction varies from unity at t = 0 to (1 + A) at long time. The following calculations indicate that the "quasisteady" calculation is but about 5% or less in error, and, thus, fully adequate for most engineering applications. For isobaric flow with $\phi \ll 1$, since $\beta \sim (Y_{Fu})^{-1}$, from Eq. 21

$$u_{u1}^{*2} \sim (Y_{Fu1})^{\nu_F - 1}\ \beta_1^{-(\nu_F+1)}\ \exp(-\beta_1) \Longrightarrow \tag{81}$$

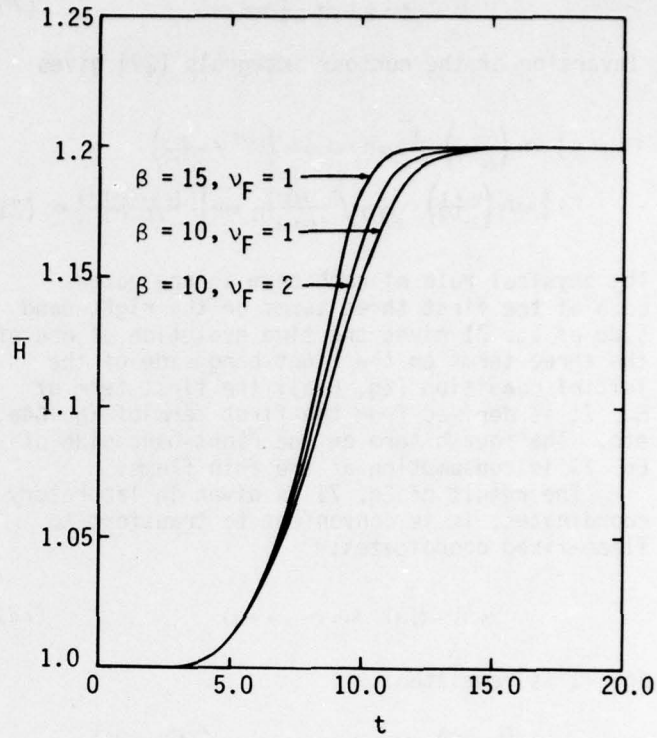

Fig. 2a - From Volterra-integral-equation formulation of thin flame propagation through a stratification in stoichiometric ratio of the unburned premixture, the dimensionless flame temperature $\overline{H}$ as a function of time t, for values of the dimensionless activation temperature β and stoichiometric coefficient for fuel ν_F. Here, Le = 1, A = 0.2, L = 10. It may be noted that $\overline{H}(0) = 1$

$$\left(\frac{u_{u2}^*}{u_{u1}^*}\right) = \left(\frac{Y_{Fu2}}{Y_{Fu1}}\right)^{(\nu_F-1)/2} \left(\frac{\beta_1}{\beta_2}\right)^{(\nu_F+1)/2} \exp\left\{\frac{\beta_1}{2}\left(1 - \frac{\beta_2}{\beta_1}\right)\right\} \Longrightarrow \tag{82a}$$

$$\left(\frac{u_{u2}^*}{u_{u1}^*}\right) = \left(\frac{Y_{Fu2}}{Y_{Fu1}}\right)^{\nu_F} \exp\left\{\frac{\beta_1}{2}\left(1 - \frac{Y_{Fu1}}{Y_{Fu2}}\right)\right\} \tag{82b}$$

since $(\beta_2/\beta_1) = (Y_{Fu1}/Y_{Fu2})$. Subscript 1 denotes the initial condition (for which the upwind asymptotic value of the mass fraction $Y_{Fu1} = 1$); subscript 2 denotes the effective upwind asymptotic value of Y_{Fu} at some later time. Since m'(t) is a dimensionless flame speed relative to the gas, for fixed cold-premixture density,

$$\frac{m_2'}{m_1'} = \left(\frac{Y_{Fu2}}{Y_{Fu1}}\right)^{\nu_F} \exp\left[\frac{\beta}{2}\left(1 - \frac{Y_{Fu1}}{Y_{Fu2}}\right)\right]. \tag{82c}$$

where $m_1' = 1$. The largest (or smallest) value that the ratio (Y_{Fu2}/Y_{Fu1}) achieves is $(1 + A)$, a value independent of both L and Le; this limiting value occurs for $t \to \infty$:

$$m_2'(t \to \infty) \to (1 + A)^{\nu_F} \exp\left(\frac{\beta A}{2(1 + A)}\right). \tag{83}$$

Some appreciation for the relative roles of parameters is obtained from the following calculations (unless otherwise specified, $\beta = 10$, $\nu_F = 1$, $A = 0.2$ so $m_2'(t \to \infty) \to 2.76$): for $A = -0.2$, $m_2'(t \to \infty) \to 0.23$; for $\beta = 15$, $m_2'(t \to \infty) \to 4.19$; for $\nu_F = 2$, $m_2'(t \to \infty) \to 3.31$.

For Le = 1, an integral exists for steady laminar isobaric adiabatic flame propagation in the form $(Y + T) = \text{const.}$, where $T = 0$ at the cold boundary and $Y = 0$ at the hot boundary. Heuristically, this relation can be employed to define an instantaneously equivalent steady problem for a flame propagating through a fuel-mass-fraction gradient. Specifically, fuel mass fraction upwind, where the normalized temperature is zero, is associated with the instantaneous temperature at the flame, where the fuel mass fraction vanishes: $Y_{Fu2}(t) \equiv \bar{H}(t)$. For $t \to 0$, $Y_{Fu2} \to \bar{H}_0 \equiv 1$; for $t \to \infty$, $Y_{Fu2} \to \bar{H}(t \to \infty) \equiv (1 + A)$. With $F_{Fu2} \equiv \bar{H}(t)$, a "quasisteady" m_2' may be computed from Eq. 82c to compare with the instantaneous m_2' calculated from the two simultaneous integral equations. For the parameter ranges $\beta = O(10)$, $\nu_F = O(1)$, $A = O(10^{-1})$, the flame speed m' is underestimated by no more than 6% by the "quasisteady" approach.

For Le = O(1), the equivalency $F_{Fu2}(t) \equiv \bar{H}(t)$ may be defined again for purposes of comparing a "quasisteady" flame speed with the instantaneous m_2' calculated from solution of a flame propagating through a premixture of nonuniform stoichiometry. The cited integral, $(Y + T) = \text{const.}$, no longer holds, so that the concept that, in steady laminar adiabatic isobaric flame propagation, the hot-boundary temperature achieved from a given cold-boundary premixture is independent of Lewis-Semenov number, is employed. However, as Le departs from unity, the accuracy degenerates.

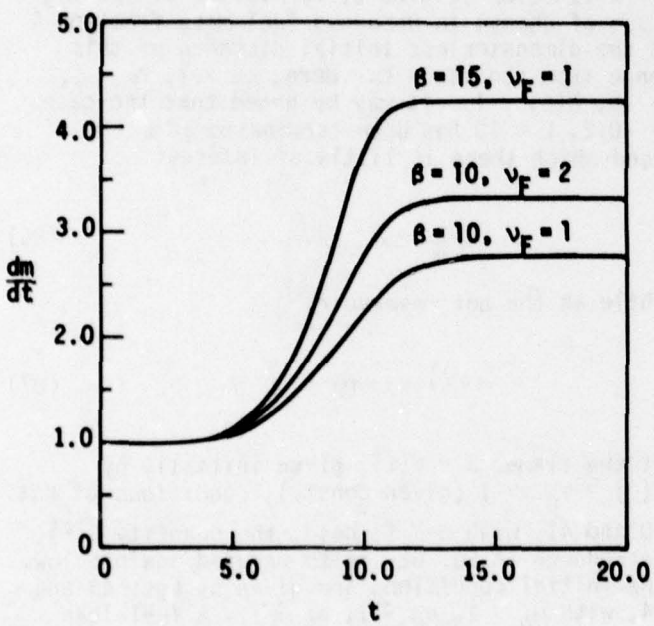

Fig. 2b - From Volterra-integral-equation formulation of thin-flame propagation through a stratification in stoichiometric ratio of the *unburned premixture*, the dimensionless time rate of change of the flame position in von Mises coordinates dm/dt as a function of time t, for values of the dimensionless activation temperature β and stoichiometric coefficient for fuel ν_F. Here, Le = 1, A = 0.2, L = 10. It may be noted that $\bar{H}(0) = 1$

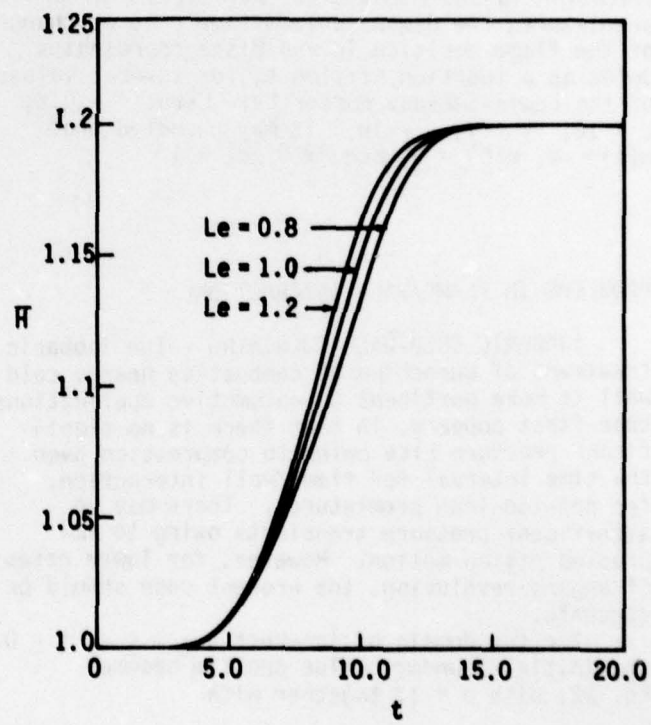

Fig. 3a - From Volterra-integral-equation formulation of thin-flame propagation through a stratification in stoichiometric ratio of the unburned premixture, the dimensionless flame temperature $\bar{H}$ as a function of time t, for several values of the Lewis-Semenov number Le. Here, A = 0.2, L = 10, $\nu_F = 1$, $\beta = 10$. It may be noted that $\bar{H}(0) = 1$

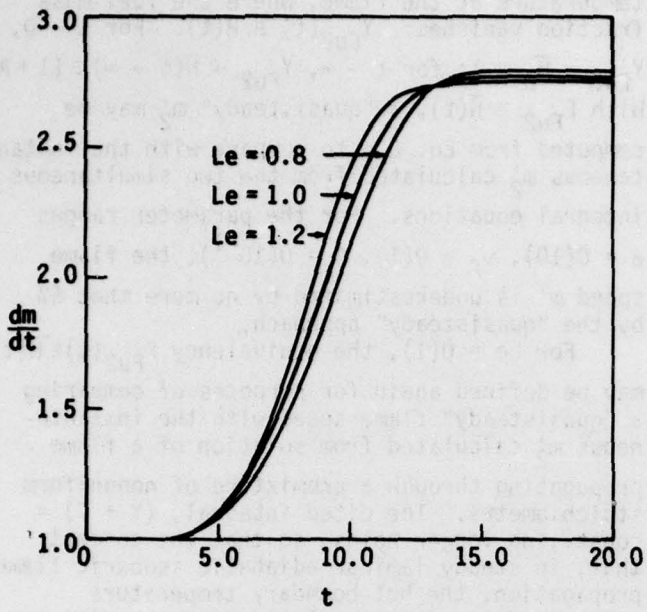

Fig. 3b - From Volterra-integral-equation formulation of thin-flame propagation through a stratification in stoichiometric ratio of the unburned premixture, the dimensionless time rate of change of the flame position in von Mises coordinates dm/dt as a function of time t, for several values of the Lewis-Semenov number Le. Here, A = 0.2, L = 10, $\nu_F = 1$, $\beta = 10$. It may be noted that $m(t) = -\Psi$, $m(0) = 0$, and $dm(0)/dt = 1$

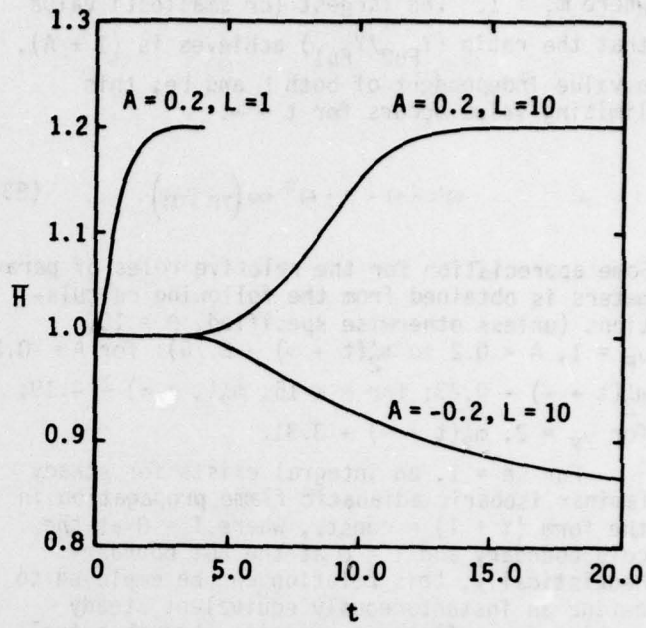

Fig. 4a - From Volterra-integral-equation formulation of thin-flame propagation through a stratification in stoichiometric ratio of the unburned premixture, the dimensionless flame temperature $\bar{H}$ as a function of time t, for values of the magnitude of change in unburned fuel mass fraction A and the dimensionless initial distance of this change from the flame L. Here, Le = 1, $\nu_F = 1$, $\beta = 10$, $\bar{H}(0) = 1$. It may be noted that the case A = -0.2, L = 10 has been terminated at a time beyond which there is little of interest

PROBLEMS IN FLAME/WALL INTERACTION

ISOBARIC COLD-WALL QUENCHING - The isobaric treatment of quenching of combustion near a cold wall is more pertinent to automotive applications than first appears, in that there is no significant pressure rise owing to compression over the time interval for flame/wall interaction, for not-too-lean premixtures. There may be significant pressure transients owing to impressed piston motion. However, for lower rates of engine revolution, the present case should be adequate.

For the domain of interest $0 \leq \psi \leq \infty$, $t \geq 0$, the initial/boundary value problem becomes Eq. 22, with p = 1, together with

$$Y \equiv 0, \ \frac{\partial h}{\partial t} - Le\,\frac{\partial^2 h}{\partial \psi^2} = 0 \qquad \text{for } \Psi < \psi < \infty \ ; \tag{84}$$

$$\frac{\partial Y}{\partial t} - \frac{\partial^2 Y}{\partial \psi^2} = 0, \ \frac{\partial H}{\partial t} - Le\,\frac{\partial^2 H}{\partial \psi^2} = 0 \qquad \text{for } 0 < \psi < \Psi \ . \tag{85}$$

At the cold noncatalytic wall, the boundary conditions are

$$H \to 0, \ \frac{\partial Y}{\partial \psi} \to 0 \text{ as } \psi \to 0 \text{ (for } t \geq 0), \tag{86}$$

while at the hot reservoir,

$$h \to 1 \text{ as } \psi \to \infty \text{ (for } t \geq 0). \tag{87}$$

At the flame, $\psi = \Psi(t)$, given initially by $\Psi(0) \equiv \Psi_0 >> 1$ (given const.), conditions of Eqs. 40 and 41, with p = 1, hold; the quantity F(t), introduced in Eq. 62, is to be used again below. The initial conditions are given by Eqs. 43 and 44, with $\bar{H}_0 = 1$, $d_0 \doteq 1$, $b_0 \doteq 1$. A fuel-lean thin vigorous flame, initially far from the cold impervious noncatalytic wall, propagates towards the wall and interacts with it.

<u>Derivation of Volterra Integral Equations by Integral Transform</u> - First, the integral-equation reduction to a problem in time only is executed. The semi-infinite domain in ψ is extended to the full-infinite domain via odd symmetry for the temperature, and even symmetry for the fuel mass fraction, about $\psi = 0$; the boundary conditions at the thin flame $\psi = \Psi(t)$

are incorporated in the partial differential equations by use of the Dirac-delta function, as was done earlier. Hence,

$$\frac{\partial Y}{\partial t} - \frac{\partial^2 Y}{\partial \psi^2} = -F\delta[\psi - \Psi] - F\delta[\psi + \Psi]. \tag{88}$$

$$\frac{\partial T}{\partial t} - Le\,\frac{\partial^2 T}{\partial \psi^2} = F\delta[\psi - \Psi] - F\delta[\psi + \Psi]. \tag{89}$$

Application of the Fourier integral transform over ψ is now straightforward. However, the initial conditions must be modified slightly to preserve the even symmetry of $Y(\psi,t)$, and the odd symmetry of $T(\psi,t)$. Here, it is taken that, as $t \to 0$,

$$Y_0 \to \begin{cases} 0 & \text{for } |\psi| > \Psi_0 \\ \dfrac{\cosh(\alpha\,\Psi_0) - \cosh(\alpha\,\psi)}{\cosh(\alpha\,\Psi_0) - 1} & \text{for } |\psi| < \Psi_0, \end{cases} \tag{90}$$

$$T_0 \to \begin{cases} 1 & \text{for } |\psi| > \Psi_0 \\ \dfrac{\sinh(\beta\,\psi)}{\sinh(\beta\,\Psi_0)} & \text{for } |\psi| < \Psi_0, \end{cases} \tag{91}$$

where α,β are constants to be assigned, such that these forms simulate initial conditions at the flame front ($\psi \to \Psi_{0-}$) as closely as possible. Satisfaction of the boundary conditions for $\psi \to \Psi_{0-}$ for an adiabatic flame gives

$$\frac{dY_0}{d\psi} \to -1 \longrightarrow \frac{\alpha\,\sinh(\alpha\,\Psi_0)}{\cosh(\alpha\,\Psi_0)-1} = 1\,; \tag{92}$$

$$Le\,\frac{dT_0}{d\psi} \to 1 \longrightarrow \beta\,\coth(\beta\,\Psi_0) = \frac{1}{Le}\,. \tag{93}$$

For $\Psi_0 \gg 1$,

$$\alpha \approx 1,\ \beta \approx \frac{1}{Le}\,; \tag{94}$$

Also, $T_0(\psi)$ and $Y_0(\psi)$ are virtually identical to the initial profiles first discussed.

As before, the Fourier transform of Eq. 88 over ψ yields formally

$$\frac{\partial \bar{Y}}{\partial t} - s^2\,\bar{Y} = -F\left[e^{-s\Psi} + e^{s\Psi}\right] \longrightarrow \tag{95}$$

$$\bar{Y}(s,t) = \bar{Y}(s,0)\,\exp(s^2 t)$$

$$- \int_0^t F(t')\left\{\exp[s^2(t-t')]\right\}\left\{\exp[-s\Psi(t')] + \exp[s\Psi(t')]\right\} dt'. \tag{96}$$

But, from Eq. 90, with $A = \cosh(\alpha\Psi_0)/[\cosh(\alpha\Psi_0)-1]$,

$$\bar{Y}(s,0) = 2A\left\{\frac{\sinh(s\,\Psi_0)}{s} - \frac{\sinh[(s-\alpha)\,\Psi_0]}{2(s-\alpha)\,\cosh(\alpha\,\Psi_0)} - \frac{\sinh[(s+\alpha)\,\Psi_0]}{2(s+\alpha)\,\cosh(\alpha\,\Psi_0)}\right\}. \tag{97}$$

Insertion of Eq. 97 in Eq. 96 and inverting gives

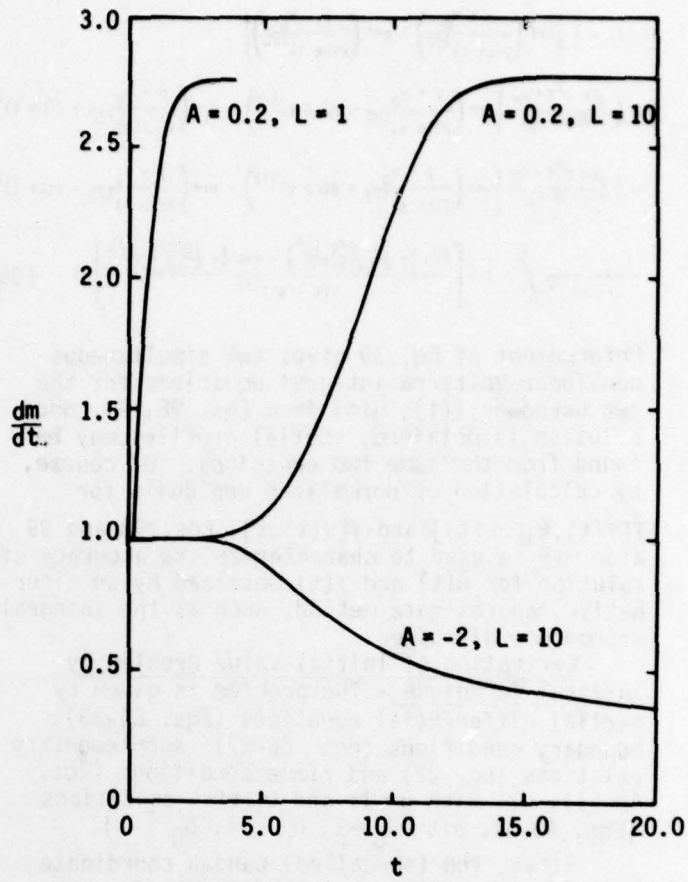

Fig. 4b - From Volterra-integral equation formulation of thin-flame propagation through a stratification in stoichiometric ratio of the unburned premixture, the dimensionless time rate of change of the flame position in von Mises coordinates dm/dt as a function of time t, for values A and L. Here, Le = 1, ν_F = 1, β = 10, m(0) = 0, dm(0)/dt = 1. It may be noted that the case A = -0.2, L = 10 has been terminated at a time beyond which there is little of interest

$$\begin{aligned} Y(\psi,t) = A\Bigg(&\frac{1}{2}\left[\mathrm{erf}\left(\frac{\psi+\Psi_0}{2t^{1/2}}\right) - \mathrm{erf}\left(\frac{\psi-\Psi_0}{2t^{1/2}}\right)\right] \\ &- \frac{1}{4}\,\frac{e^{\alpha^2 t+\alpha\psi}}{\cosh(\alpha\Psi_0)}\left[\mathrm{erf}\left(\frac{\psi+\Psi_0}{2t^{1/2}} + \alpha t^{1/2}\right) - \mathrm{erf}\left(\frac{\psi-\Psi_0}{2t^{1/2}} + \alpha t^{1/2}\right)\right] \\ &- \frac{1}{4}\,\frac{e^{\alpha^2 t-\alpha\psi}}{\cosh(\alpha\Psi_0)}\left[\mathrm{erf}\left(\frac{\psi+\Psi_0}{2t^{1/2}} - \alpha t^{1/2}\right) - \mathrm{erf}\left(\frac{\psi-\Psi_0}{2t^{1/2}} - \alpha t^{1/2}\right)\right]\Bigg) \\ &- \frac{1}{2\pi^{1/2}}\int_0^t F(t')\left[\frac{\exp\left\{-\frac{(\psi-\Psi(t'))^2}{4(t-t')}\right\} + \exp\left\{-\frac{(\psi+\Psi(t'))^2}{4(t-t')}\right\}}{(t-t')^{1/2}}\right] dt' \end{aligned} \tag{98}$$

The terms which multiply A describe the time evolution of the initial conditions, while the integral term describes chemical consumption. Similarly,

$$T(\psi,t) = \frac{1}{2}\left\{\mathrm{erf}\left(\frac{\psi+\Psi_0}{2(\mathrm{Le}\,t)^{1/2}}\right) + \mathrm{erf}\left(\frac{\psi-\Psi_0}{2(\mathrm{Le}\,t)^{1/2}}\right)\right\}$$

$$+ \frac{1}{4}\frac{e^{\mathrm{Le}\,\beta^2 t+\beta\psi}}{\sinh(\beta\Psi_0)}\left[\mathrm{erf}\left(\frac{\psi+\Psi_0}{2(\mathrm{Le}\,t)^{1/2}} + \beta(\mathrm{Le}\,t)^{1/2}\right) - \mathrm{erf}\left(\frac{\psi-\Psi_0}{2(\mathrm{Le}\,t)^{1/2}} + \beta(\mathrm{Le}\,t)^{1/2}\right)\right]$$

$$- \frac{1}{4}\frac{e^{\mathrm{Le}\,\beta^2 t-\beta\psi}}{\sinh(\beta\Psi_0)}\left[\mathrm{erf}\left(\frac{\psi+\Psi_0}{2(\mathrm{Le}\,t)^{1/2}} - \beta(\mathrm{Le}\,t)^{1/2}\right) - \mathrm{erf}\left(\frac{\psi-\Psi_0}{2(\mathrm{Le}\,t)^{1/2}} - \beta(\mathrm{Le}\,t)^{1/2}\right)\right]$$

$$+ \frac{1}{2(\pi\mathrm{Le})^{1/2}}\int_0^t F(t')\left[\frac{\exp\left\{-\frac{(\psi-\Psi(t'))^2}{4\,\mathrm{Le}(t-t')}\right\} - \exp\left\{-\frac{(\psi+\Psi(t'))^2}{4\,\mathrm{Le}(t-t')}\right\}}{(t-t')^{1/2}}\right]dt'. \quad (99)$$

Enforcement of Eq. 39 gives two simultaneous nonlinear Volterra integral equations for the two unknowns $\Psi(t)$, $\overline{H}(t)$ from Eqs. 98, 99; once solution is obtained, spatial profiles may be found from the same two equations. Of course, by calculation of normalized residuals for $T[\Psi(t),t][=\overline{H}(t)]$ and $Y[\Psi(t),t]$, Eqs. 98 and 99 also may be used to characterize the accuracy of solution for $\overline{H}(t)$ and $\Psi(t)$ obtained by an alternative, approximate method, such as the integral method now discussed.

Derivation of Initial-Value Problem by Integral Technique - The problem is given by partial differential equations (Eqs. 84-85); boundary conditions (eqs. 86-87); supplementary relations (Eq. 22) and flame conditions (Eqs. 40-41), all with $p = 1$; and initial conditions (Eqs. 43-44, with $\overline{H}_0 = 1$, $d_0 \doteq 1$, $b_0 \doteq 1$).

First, the (so-called) Landau coordinate transformation [30] is introduced to fix the flame position:

$$(\psi,t) \to (\sigma,t), \text{ with } \sigma = \psi/\Psi(t). \quad (100)$$

The initial/boundary-value problem for $Y(\sigma,t)$, $h(\sigma,t)$, $H(\sigma,t)$ is restated (here primes denote ordinary derivatives with respect to time, denoted by t):

$$Y \equiv 0,\ \frac{\partial h}{\partial t} - \frac{\Psi'}{\Psi}\sigma\frac{\partial h}{\partial\sigma} - \frac{\mathrm{Le}}{\Psi^2}\frac{\partial^2 h}{\partial\sigma^2} = 0 \quad \text{for } 1 < \sigma < \infty; \quad (101)$$

$$\frac{\partial Y}{\partial t} - \frac{\Psi'}{\Psi}\sigma\frac{\partial Y}{\partial\sigma} - \frac{1}{\Psi^2}\frac{\partial^2 Y}{\partial\sigma^2} = 0,\ \frac{\partial H}{\partial t} - \frac{\Psi'}{\Psi}\sigma\frac{\partial H}{\partial\sigma} - \frac{\mathrm{Le}}{\Psi^2}\frac{\partial^2 H}{\partial\sigma^2} = 0 \quad \text{for } 0 < \sigma < 1. \quad (102)$$

The boundary conditions, for a cold isothermal noncatalytic wall, and for the far field, are

$$H \to 0,\ \frac{\partial Y}{\partial\sigma} \to 0 \text{ as } \sigma \to 0 \text{ (for } t \geq 0);\ h \to 1 \text{ as } \sigma \to \infty \text{ (for } t \geq 0). \quad (103)$$

The conditions at the flame, $\sigma = 1$, are:

$$h \to \overline{H},\ H \to \overline{H},\ Y \to 0, \quad (104)$$

$$\left[\left(\frac{\partial Y}{\partial\sigma} + \mathrm{Le}\frac{\partial H}{\partial\sigma}\right) - \mathrm{Le}\frac{\partial h}{\partial\sigma}\right] \to 0, \text{ with } \frac{\partial Y}{\partial\sigma} = -\Psi\overline{H}^{\nu_F+1}\exp\left\{-\frac{\beta}{2}\frac{1-\overline{H}}{\overline{H}}\right\}, \text{ as } \sigma \to 1 \text{ (for } t \geq 0). \quad (105)$$

The initial conditions are, for $\overline{H}(0) \equiv \overline{H}_0 = 1$, $\Psi(0) \equiv \Psi_0 >> 1$:

$$h \to h_0 = 1 \text{ as } t \to 0 \text{ (for } 1 < \sigma < \infty); \quad (106)$$

$$H \to H_0 = \exp\{-\Psi_0(1-\sigma)/\mathrm{Le}\},\ Y \to Y_0 = [1 - \exp\{-\Psi_0(1-\sigma)\}] \text{ as } t \to 0 \text{ (for } 0 \leq \sigma \leq 1). \quad (107)$$

For $\Psi_0 >> 1$, as noted previously, these conditions are compatible with the boundary conditions to within (exponentially) small error.

The following representations of the dependent variables are taken to be good approximations for all time:

$$h(\sigma,t) = 1 - \left(1 - \overline{H}(t)\right)\exp\left\{-\frac{\Psi(t)(\sigma-1)}{\mathrm{Le}\,c(t)}\right\} \quad \text{for } 1 \leq \sigma \leq \infty; \quad (108)$$

$$H(\sigma,t) = \overline{H}(t)\frac{\sinh\left\{\frac{\Psi(t)\,\sigma}{\mathrm{Le}\,b(t)}\right\}}{\sinh\left\{\frac{\Psi(t)}{\mathrm{Le}\,b(t)}\right\}} \quad (109)$$

$$Y(\sigma,t) = 1 - \frac{\cosh\left\{\frac{\Psi(t)\sigma}{d(t)}\right\}}{\cosh\left\{\frac{\Psi(t)}{d(t)}\right\}} \quad \text{for } 0 \leq \sigma \leq 1. \quad (110)$$

For $b(0) \equiv b_0 \doteq 1$, $d(0) \equiv d_0 \doteq 1$, these adopted forms are closely compatible with the initial conditions. The two flame conditions at $\sigma = 1$ involving gradients, and the three partial differential equations, yield five relations for the five unknown functions of time $b(t)$, $c(t)$, $d(t)$, $\overline{H}(t)$, $\Psi(t)$. Initial values are:

$$\overline{H}(0) \equiv \overline{H}_0 = 1,\ \Psi(0) \equiv \Psi_0 >> 1, \text{ given const.};\ c(0) \equiv c_0 = 1 \text{ (formally)}. \quad (111)$$

The values of $b(0) \equiv b_0$, $d(0) \equiv d_0$ are to be in the manner now described.

The flame conditions (Eq. 105) give

$$-\frac{\tanh(\Psi/d)}{d} + \frac{\bar{H}}{b\tanh(\Psi/Le\,b)} - \frac{(1-\bar{H})}{c} = 0; \tag{112}$$

$$\frac{\tanh(\Psi/d)}{d} = \bar{H}^{\nu_F+1}\exp\left\{-\frac{\beta}{2}\frac{(1-\bar{H})}{\bar{H}}\right\}. \tag{113}$$

At $t = 0$, for $\Psi_0 >> 1$, these give $b_0 \approx d_0 \approx 1$ by inspection. Differentiation with respect to time gives for Eqs. 112 and 113, respectively,

$$\left[\bar{H}\left\{\frac{(\Psi/Le\,b)}{\sinh^2(\Psi/Le\,b)} - \frac{1}{\tanh(\Psi/Le\,b)}\right\}\right]\frac{b'}{b^2} + (1-\bar{H})\frac{c'}{c^2}$$
$$+\left[\tanh(\Psi/d) + \frac{(\Psi/d)}{\cosh^2(\Psi/d)}\right]\frac{d'}{d^2} - \left[\frac{(\Psi/d)}{d\cosh^2(\Psi/d)} + \frac{\bar{H}(\Psi/Le\,b)}{b\sinh^2(\Psi/Le\,b)}\right]\frac{\Psi'}{\Psi}$$
$$+\left[\bar{H}\left\{\frac{1}{b\tanh(\Psi/Le\,b)} + \frac{1}{c}\right\}\right]\frac{\bar{H}'}{\bar{H}} = 0; \tag{114}$$

$$-\left[1 + \frac{(\Psi/d)}{\sinh(\Psi/d)\cosh(\Psi/d)}\right]\frac{d'}{d} + \left[\frac{(\Psi/d)}{\sinh(\Psi/d)\cosh(\Psi/d)}\right]\frac{\Psi'}{\Psi}$$
$$-\left[(\nu_F + 1) + \frac{\beta}{2\bar{H}}\right]\frac{\bar{H}'}{\bar{H}} = 0. \tag{115}$$

In general, the partial differential equations may be integrated with respect to σ, upon imposition of the boundary conditions and of the flame conditions, to yield

$$\frac{d(\Psi\Theta)}{dt} = \frac{1}{\Psi}\left(\frac{\partial Y}{\partial\sigma}\right)_f$$
$$\text{where } \Theta = \int_0^1 Y\,d\sigma,\ \text{fcn}(t),\ \left(\frac{\partial Y}{\partial\sigma}\right)_f = \frac{\partial Y}{\partial\sigma}(1,t),\ \text{fcn}(t); \tag{116}$$

$$\frac{d(\Psi\Phi)}{dt} = \frac{Le}{\Psi}\left[\left(\frac{\partial H}{\partial\sigma}\right)_f - \left(\frac{\partial H}{\partial\sigma}\right)_w\right] + \bar{H}\frac{d\Psi}{dt}.$$
$$\text{where } \Phi = \int_0^1 H\,d\sigma,\ \text{fnc}(t),\ \left(\frac{\partial H}{\partial\sigma}\right)_f = \frac{\partial H}{\partial\sigma}(1,t),\ \text{fnc}(t),\ \left(\frac{\partial H}{\partial\sigma}\right)_w = \frac{\partial H}{\partial\sigma}(0,t),\ \text{fcn}(t); \tag{117}$$

$$\frac{d(\Psi\Pi)}{dt} = \frac{Le}{\Psi}\left(\frac{\partial h}{\partial\sigma}\right)_f - (1-\bar{H})\frac{d\Psi}{dt}.$$
$$\text{where } \Pi = \int_1^\infty (1-h)\,d\sigma,\ \text{fnc}(t),\ \left(\frac{\partial h}{\partial\sigma}\right)_f = \frac{\partial h}{\partial\sigma}(1,t),\ \text{fnc}(t). \tag{118}$$

For the specific forms adopted,

$$\Theta = 1 - \frac{\tanh(\Psi/d)}{(\Psi/d)},\ \left(\frac{\partial Y}{\partial\sigma}\right)_f = -\left(\frac{\Psi}{d}\right)\tanh(\Psi/d); \tag{119}$$

$$\Phi = \frac{\bar{H}[\cosh(\Psi/Le\,b) - 1]}{(\Psi/Le\,b)\sinh(\Psi/Le\,b)},\ \left(\frac{\partial H}{\partial\sigma}\right)_f = \bar{H}\frac{(\Psi/Le\,b)}{\tanh(\Psi/Le\,b)},\ \left(\frac{\partial H}{\partial\sigma}\right)_w = \bar{H}\frac{(\Psi/Le\,b)}{\sinh(\Psi/Le\,b)}; \tag{120}$$

$$\Pi = \frac{(1-\bar{H})}{(\Psi/Le\,c)},\ \left(\frac{\partial h}{\partial\sigma}\right)_f = (1-\bar{H})(\Psi/Le\,c). \tag{121}$$

Hence, from Eqs. 116 and 117

$$[(\Psi/d)\,\text{sech}^2(\Psi/d) - \tanh(\Psi/d)]d' + [\tanh^2(\Psi/d)]\Psi' = -\frac{\tanh(\Psi/d)}{d}; \tag{122}$$

$$\left[1 - \frac{(\Psi/Le\,b)}{\sinh(\Psi/Le\,b)}\right]b' - \left[\frac{1}{Le\tanh(\Psi/Le\,b)}\right]\Psi' + \left[\frac{b}{\bar{H}}\right]\bar{H}' = \frac{1}{Le\,b}; \tag{123}$$

and from Eq. 118

$$(1-\bar{H})c' + \frac{(1-\bar{H})}{Le}\Psi' - c\,\bar{H}' = \frac{1-\bar{H}}{Le\,c}. \tag{124}$$

This last equation states that, if $\bar{H}_0 = 1$, $\bar{H} = 1$ at all subsequent time; this artifact of the approximate procedure is circumvented by starting with a value of $\bar{H}$ slightly displaced from unity. The fact that the calculational procedure tends to establish a steady propagating flame while still away from the wall ($\Psi >> 1$), provided $\bar{H}_0$ is not too far from unity, is established in the section on the effects of transients on flame propagation.

Equations 114-115, 122-124, subject to the initial conditions implicit in Eqs. 111-113, constitute the sought-after initial-value problem for $b(t)$, $c(t)$, $d(t)$, $\bar{H}(5)$, $\Psi(t)$. Substitution of the results in Eqs. 108-110, 22 gives the solution for $Y(\psi,t)$, $T(\psi,t)$, $\Psi(t)$; results depend on the parameters K, β, ν_F, and Le. (Ψ_0, c_0, $\bar{H}_0$ must also be selected, but there is minor sensitivity to these quantities introduced by the method of solution.) (See Figs. 5-8.)

Other output quantities of interest are the rate of fuel consumption at the flame (i.e., the derivative of the fuel mass fraction at the flame), the fuel mass fraction at the wall, and the temperature gradient at the wall; these quantities are, respectively (if $X_f(t)$ is the site in the Cartesian coordinate of the flame $\Psi(t)$):

$$\left(\frac{\partial Y}{\partial \sigma}\right)_f = -(\Psi/d)\tanh(\Psi/d) \longrightarrow \left(\frac{\partial Y}{\partial \psi}\right)_f = -(1/d)\tanh(\Psi/d) \longrightarrow$$

$$\left(\frac{\partial Y}{\partial x}\right)_f = -\frac{(1/d)\tanh(\Psi/d)}{(1+K\bar{H})}\,; \tag{125}$$

$$Y_w = \frac{\cosh(\Psi/d) - 1}{\cosh(\Psi/d)}\,; \tag{126}$$

$$\left(\frac{\partial H}{\partial \sigma}\right)_w = \bar{H}\,\frac{(\Psi/Le\ b)}{\sinh(\Psi/Le\ b)} \longrightarrow \left(\frac{\partial H}{\partial \psi}\right)_w = \bar{H}\,\frac{(1/Le\ b)}{\sinh(\Psi/Le\ b)} \longrightarrow$$

$$\left(\frac{\partial H}{\partial x}\right)_w = \bar{H}\,\frac{(1/Le\ b)}{\sinh(\Psi/Le\ b)}\,. \tag{127}$$

The association of Cartesian and von Mises coordinates is

$$x = \begin{cases} \Psi\left(\sigma + \dfrac{K\,\bar{H}[\cosh(\Psi\sigma/Le\ b) - 1]}{(\Psi/Le\ b)\sinh(\Psi/Le\ b)}\right) & \text{for } 0 \le \sigma \le 1 \\ X_f + \Psi\left((K+1)(\sigma-1) - \dfrac{K(1-\bar{H})\,[1-\exp(-\Psi(\sigma-1)/Le\ c)]}{(\Psi/Le\ c)}\right) & \text{for } 1 \le \sigma \le \infty, \end{cases} \tag{128}$$

where $X_f(t)$ is given by

$$X_f = \Psi\int_0^1 (1 + K\,H)d\sigma = \Psi\left(1 + \frac{K\,\bar{H}[\cosh(\Psi/Le\ b) - 1]}{(\Psi/Le\ b)\sinh(\Psi/Le\ b)}\right). \tag{129}$$

Adoption of a thin-flame model furnishes a natural and an explicit definition of quench-layer thickness. The rate of change of the flame position with time in the Cartesian coordinate is

$$U_f \equiv \frac{dX_f}{dt} = X_f' = (1 + K\,\bar{H})\Psi' + \frac{K\,\bar{H}[\cosh(\Psi/Le\ b) - 1]}{b\sinh(\Psi/Le\ b)}\,. \tag{130}$$

The gas speed at the flame is

$$u_f = \left(\frac{\partial x(\Psi, t)}{\partial t}\right)_\psi = K\int_0^\Psi \frac{\partial H}{\partial t}\,d\psi = \frac{K\,Le}{\Psi}\left[\left(\frac{\partial H}{\partial \sigma}\right)_f - \left(\frac{\partial H}{\partial \sigma}\right)_w\right]$$

$$= \frac{K\,\bar{H}[\cosh(\Psi/Le\ b) - 1}{b\sinh(\Psi/Le\ b)}\,. \tag{131}$$

Thus, the speed of the flame relative to the speed of the gas at the flame, $(U_f - u_f)$ is $(1 + K\bar{H})\Psi'$. Initially, for $\Psi \gg 1$, $H \doteq 1$, and $\Psi' \doteq -1$, so $U_f \doteq -1$ and $u_f \doteq K$. Finally, a quantity defined to be the net remaining fuel, $N(t)$, is introduced

$$N \equiv \int_0^{X_f} \rho Y\,dx = \Psi\int_0^1 Y\,d\sigma$$

$$= \Psi - d\tanh(\Psi/d)\,, \tag{132}$$

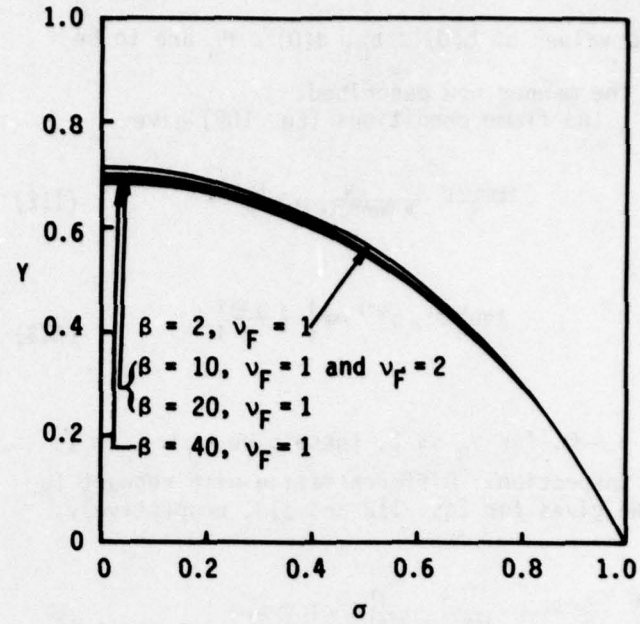

Fig. 5a - From integral-method results for a cold wall (at temperature T = 0), profiles for the mass fraction Y as a function of the coordinate $\sigma[=\psi/\Psi(t)]$ at time t = 8.04, for several values of the dimensionless Arrhenius activation temperature β. Here, K = 6, Le = 1, ν_F = 1, and the initial time is defined by $\Psi(t = 0) = \Psi_0 = 10$. This is the first of five figures which describe the augmented quenching for flame interaction with a cold wall with increase of the activation temperature β

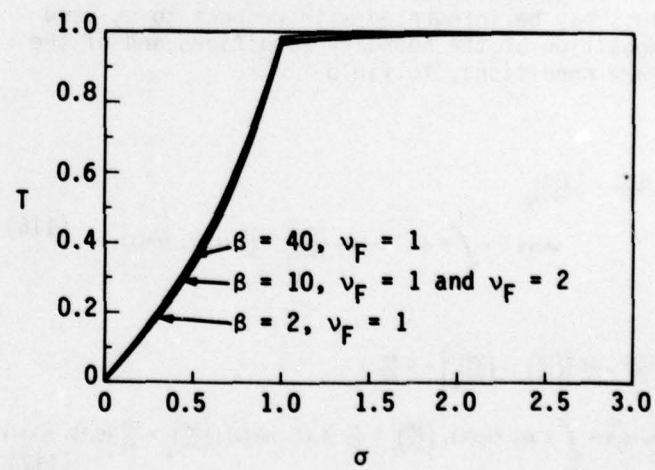

Fig. 5b - From integral-method results for a cold wall (at temperature T = 0), profiles for the temperature T as a function of the coordinate $\sigma[=\psi/\Psi(t)]$ at time t = 8.04, for several values of the dimensionless Arrhenius activation temperature β. Here, K = 6, Le = 1, ν_F = 1, and the initial time is defined by $\Psi(t = 0) = \Psi_0 = 10$

where the subtracted term in Eq. 132 is identified to be the depletion of fuel ahead of the flame owing to the presence of the flame.

ISOBARIC ACCELERATION TOWARD AN ADIABATIC WALL - Derivation of Volterra Integral Equations by Integral Transform - The entire derivation leading to Eq. 98 holds without modification. However, because Eq. 86 is altered to

$$\frac{\partial H}{\partial \psi} \to 0, \ \frac{\partial Y}{\partial \psi} \quad 0 \text{ as } \psi \to 0 \text{ (for } t \geq 0), \tag{133}$$

Eq. 81 is revised to

$$\frac{\partial T}{\partial t} - Le \frac{\partial^2 T}{\partial \psi^2} = F\,\delta[\psi - \Psi] + F\,\delta[\psi + \Psi], \ -\infty < \psi < \infty, \ t \geq 0, \tag{134}$$

to enforce the evenness of $T(\psi, t)$ about $\psi = 0$ for the adiabatic case. Also, Eq. 92 is revised, so that, as $t \to 0$

$$T(\psi,t) \to T_0(\psi) = \begin{cases} \dfrac{\cosh(\delta\psi) - 1}{\cosh(\delta\Psi_0) - 1} & \text{for } |\psi| < \Psi_0 \\ 1 & \text{for } |\psi| > \Psi_0 \end{cases}; \tag{135}$$

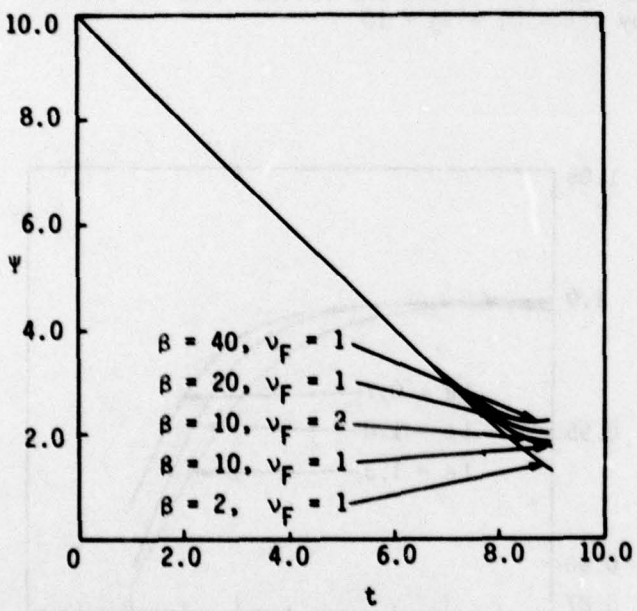

Fig. 5c - From integral-method results for a cold wall (at temperature T = 0), profiles for the position of the flame in von Mises (mass-weighted) coordinates Ψ as a function of time t, for several values of the dimensionless Arrhenius activation temperature β. Here, K = 6, Le = 1, ν_F = 1, and the initial time is defined by $\Psi(t = 0) = \Psi_0 = 10$

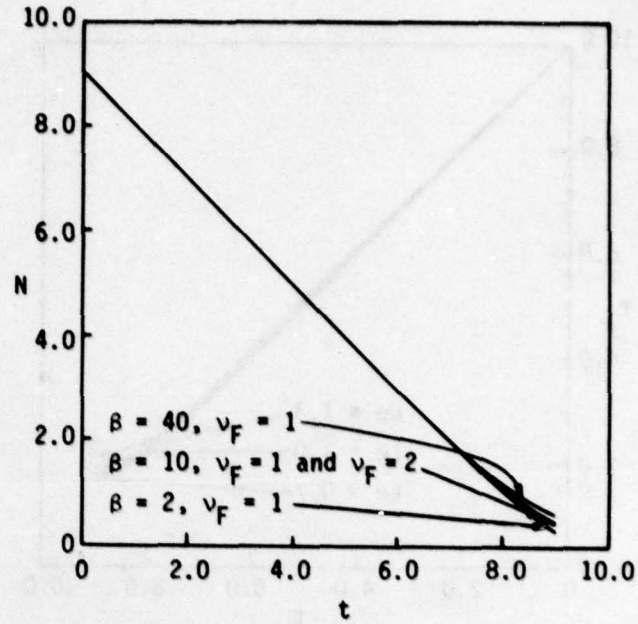

Fig. 5d - From integral-method results for a cold wall (at temperature T = 0), profiles for the net remaining fuel N (defined by Eq. 132) as a function of time t, for several values of the dimensionless activation temperature β. Here, K = 6, Le = 1, ν_F = 1, and the initial time is defined by $\Psi(t = 0) = \Psi_0 = 10$

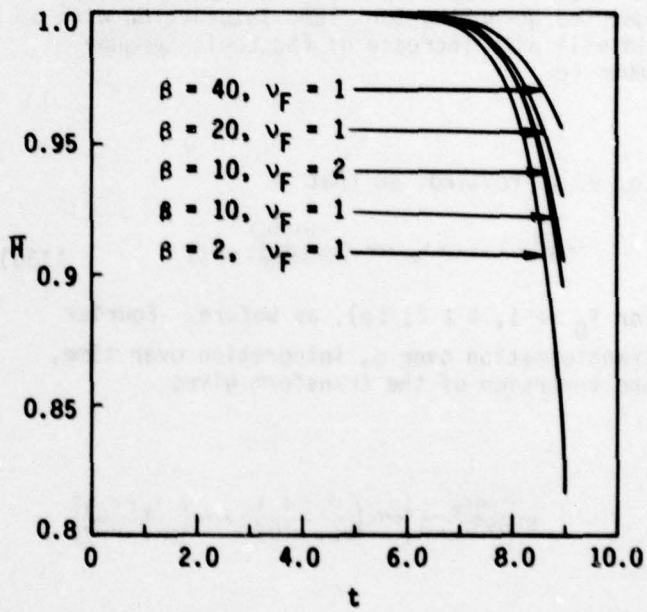

Fig. 5e - From integral-method results for a cold wall (at temperature T = 0), profiles for the flame temperature $\bar{H}$ as a function of time t, for several values of the dimensionless Arrhenius activation temperature β. Here, K = 6, Le = 1, ν_F = 1, and the initial time is defined by $\psi(t = 0) = \Psi_0 = 10$

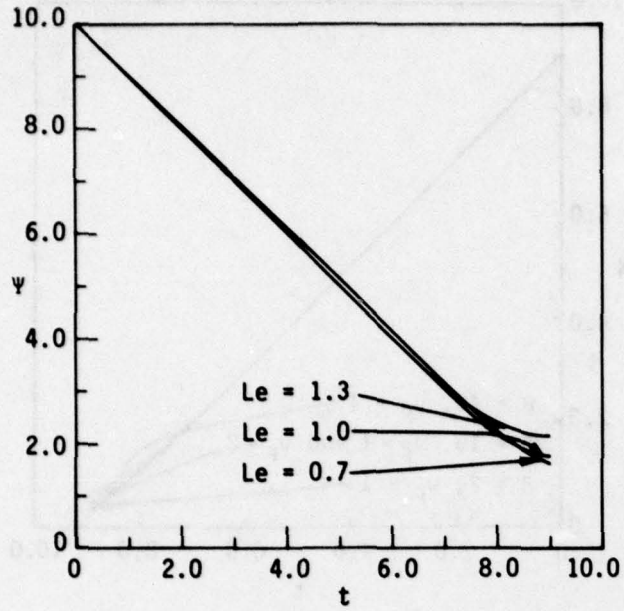

Fig. 6a - From integral-method results for a cold wall (at temperature T = 0), profiles for the position of the flame in von Mises (mass-weighted) coordinates Ψ as a function of time t, for several values of the Lewis-Semenov number Le. Here, $\beta = 10$, $K = 6$, $\nu_F = 1$, and the initial time is defined by $\Psi(t = 0) = \Psi_0 = 10$. This is the first of three figures which describe the augmented quenching for flame interaction with a cold wall with increase of the Lewis-Semenov number Le

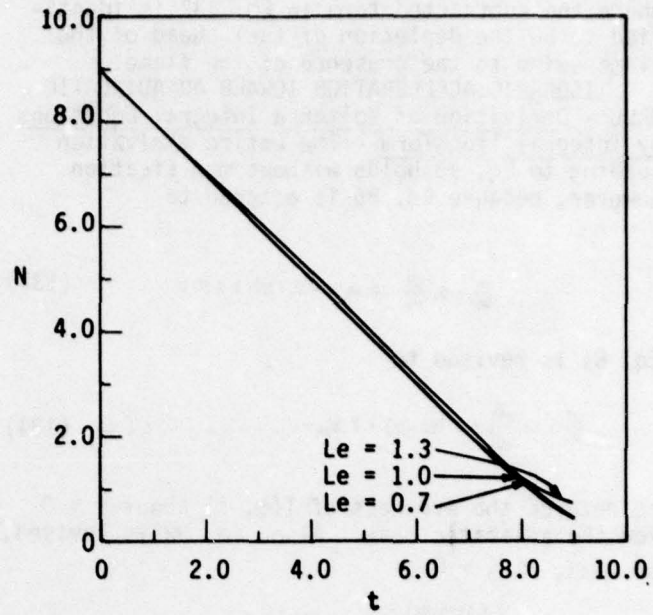

Fig. 6b - From integral-method results for a cold wall (at temperature T = 0), profiles of the net remaining fuel N (defined by Eq. 132) as a function of time t, for several values of the Lewis-Semenov number Le. Here, $\beta = 10$, $K = 6$, $\nu_F = 1$, and the initial time is defined by $\Psi(t = 0) = \Psi_0 = 10$

Eq. 93 is revised, so that

$$\mathrm{Le}\,\frac{dT_0}{d\psi} \to 1 \text{ as } \psi \to \Psi_{0-} \Longrightarrow \beta\,\frac{\sinh(\beta\Psi_0)}{\cosh(\beta\Psi_0) - 1} = \frac{1}{\mathrm{Le}}\,. \tag{136}$$

For $\Psi_0 >> 1$, $\beta \doteq (1/\mathrm{Le})$, as before. Fourier transformation over ψ, integration over time, and inversion of the transform gives

$$T(\psi,t) = \frac{\cosh(\beta\Psi_0)}{2[\cosh(\beta\Psi_0)-1]}\left[\mathrm{erfc}\left(\frac{\Psi_0+\psi}{2(\mathrm{Le}\,t)^{1/2}}\right) + \mathrm{erfc}\left(\frac{\Psi_0-\psi}{2(\mathrm{Le}\,t)^{1/2}}\right)\right]$$

$$+ \frac{e^{\mathrm{Le}\,\beta^2 t + \beta\psi}}{4[\cosh(\beta\Psi_0)-1]}\left[\mathrm{erf}\left(\frac{\psi+\Psi_0}{2(\mathrm{Le}\,t)^{1/2}} + \beta(\mathrm{Le}\,t)^{1/2}\right) - \mathrm{erf}\left(\frac{\psi-\Psi_0}{2(\mathrm{Le}\,t)^{1/2}} + \beta(\mathrm{Le}\,t)^{1/2}\right)\right]$$

$$+ \frac{e^{\mathrm{Le}\,\beta^2 t - \beta\psi}}{4[\cosh(\beta\Psi_0)-1]}\left[\mathrm{erf}\left(\frac{\Psi_0+\psi}{2(\mathrm{Le}\,t)^{1/2}} - \beta(\mathrm{Le}\,t)^{1/2}\right) - \mathrm{erf}\left(\frac{\psi-\Psi_0}{2(\mathrm{Le}\,t)^{1/2}} - \beta(\mathrm{Le}\,t)^{1/2}\right)\right]$$

$$+ \frac{1}{2(\pi\,\mathrm{Le})^{1/2}}\int_0^t F(t')\,\frac{\exp\left\{-\frac{[\psi-\Psi(t')]^2}{4\,\mathrm{Le}(t-t')}\right\} + \exp\left\{-\frac{[\psi+\Psi(t')]^2}{4\,\mathrm{Le}(t-t')}\right\}}{(t-t')^{1/2}}\,dt'. \tag{137}$$

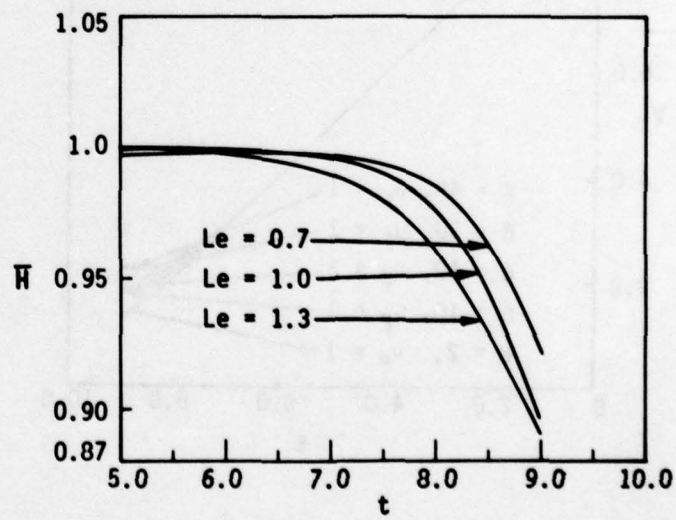

Fig. 6c - From integral-method results for a cold wall (at temperature T = 0), profiles of the thin-flame temperature $\bar{H}$ as a function of time t, for several values of the Lewis-Semenov number Le. Here, $\beta = 10$, $K = 6$, $\nu_F = 1$, and the initial time is defined by $\Psi(t = 0) = \Psi_0 = 10$

Enforcing $T[\Psi(t),t] = \overline{H}(t)$ yields an integral equation to complement the one found by enforcing $Y[\Psi(t),t] = 0$ for Eq. 98.

Derivation of Initial-Value Problem by Integral Technique - The entire discussion from Eqs. 100-110 holds unaltered, except for the temperature boundary condition at the wall; i.e., the first of Eq. 103 becomes 133, so Eq. 109 is revised to

$$H(\sigma,t) = \overline{H}(t)\,\frac{\cosh\left\{\frac{\Psi(t)\sigma}{Le\ b(t)}\right\}}{\cosh\left\{\frac{\Psi(t)}{Le\ b(t)}\right\}} \qquad \text{for } 0 \le \sigma \le 1. \tag{138}$$

Thus, Eq. 112 becomes

$$-\frac{\tanh(\Psi/d)}{d} + \frac{\overline{H}\tanh(\Psi/Le\ b)}{b} - \frac{(1-\overline{H})}{c} = 0, \tag{139}$$

so Eq. 114 becomes

$$-\left[\overline{H}\left\{\tanh(\Psi/Le\ b) + (\Psi/Le\ b)\,\mathrm{sech}^2(\Psi/Le\ b)\right\}\right]\frac{b'}{b^2} + (1-\overline{H})\,\frac{c'}{c^2}$$
$$+\left[\tanh(\Psi/d) + (\Psi/d)\,\mathrm{sech}^2(\Psi/d)\right]\frac{d'}{d^2} - \left[\frac{(\Psi/d)\,\mathrm{sech}^2(\Psi/d)}{d} - \overline{H}\,\frac{(\Psi/Le\ b)\,\mathrm{sech}^2(\Psi/Le\ b)}{b}\right]\frac{\Psi'}{\Psi}$$
$$+\left[\overline{H}\left\{\frac{\tanh(\Psi/Le\ b)}{b} + \frac{1}{c}\right\}\right]\frac{\overline{H}'}{\overline{H}} = 0. \tag{140}$$

Also, Eq. 123 must be replaced by

$$\left[1 - \frac{(\Psi/Le\ b)}{\sinh(\Psi/Le\ b)\cosh(\Psi/Le\ b)}\right]b' - \left[\frac{\tanh(\Psi/Le\ b)}{Le}\right]\Psi' + \left[\frac{b}{\overline{H}}\right]\overline{H}' = \frac{1}{Le\ b}. \tag{141}$$

After Eqs. 139 and 113 are used to assign b_0, d_0 for specified values of Le, β, ν_F, H_0, and Ψ_0, then straightforward integration in time follows by use of Eqs. 115, 140, 122, 141, and 124.

Output quantities of interest for the adiabatic wall are the rate of fuel consumption at the flame and the fuel mass fraction at the wall; these are given by Eqs. 125 and 126, respectively. The temperature at the wall is also of interest:

$$H_w = \overline{H}\ \mathrm{sech}(\Psi/Le\ b). \tag{142}$$

Since Ψ goes from Ψ_0 (>> 1) to 0, $H_w(t)$ goes from effectively zero to the temperature at the flame as the flame front accelerates towards the wall.

The association of Cartesian and von Mises coordinates is

$$x = \begin{cases} \Psi\left(\sigma + \dfrac{K\,\overline{H}\sinh(\Psi\sigma/Le\ b)}{(\Psi/Le\ b)\cosh(\Psi/Le\ b)}\right) & \text{for } 0 \le \sigma \le 1 \\ X_f + \Psi\left((K+1)(\sigma-1) - \dfrac{K(1-\overline{H})[1-\exp(-\Psi(\sigma-1)/Le\ c)]}{(\Psi/Le\ c)}\right) & \text{for } 1 \le \sigma \le \infty, \end{cases} \tag{143}$$

where $X_f(t)$ is given by

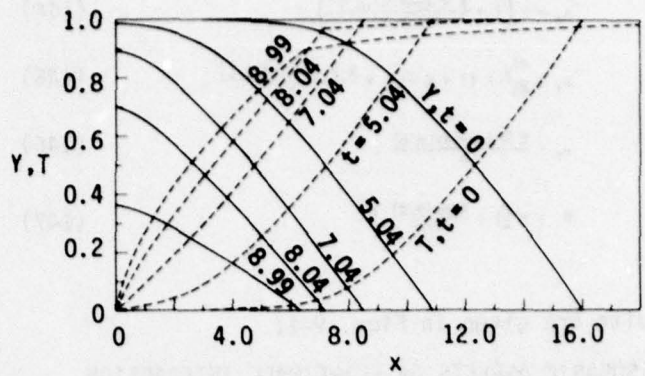

Fig. 7 - From integral-method results for a cold wall (at temperature T = 0), profiles for the (normalized, stoichiometrically adjusted) mass fraction Y and for the dimensionless temperature T as a function of the dimensionless Cartesian coordinate x, for several values of dimensionless time t. Here, β = 10, K = 6, Le = 1, ν_F = 1. The initial time corresponds to von Mises (mass-weighted) spatial coordinate $\Psi(t=0) = \Psi_0 = 10$. Whereas $\Psi'(0) = -1$, the initial flame temperature $\overline{H}(0) = 1$, and the initial net remaining fuel $N(0) = 9$, the calculation is terminated at t = 8.99 with $\Psi'(0) = 0.123$, $\overline{H} = 0.896$, and N = 0.434. The flame speed U_f increases from an initial value of -1.00 at t = 0 to a maximum value of -1.37 at t ≐ 7.42, then decreases rapidly [with $U_f(t = 8.99) = -0.372$]

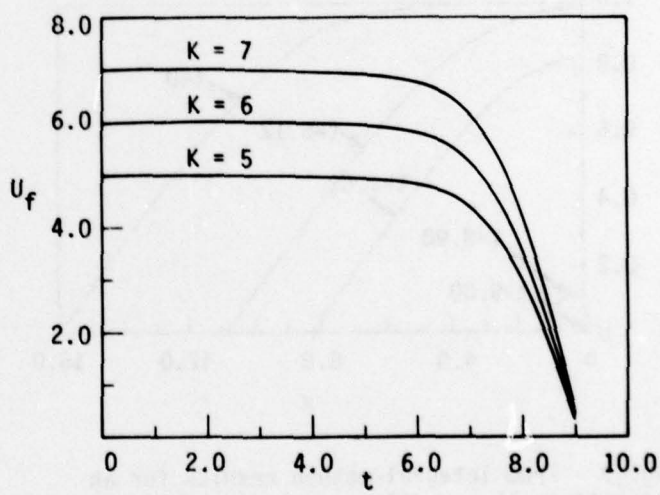

Fig. 8 - From integral-method results for a cold wall (at temperature T = 0), the speed of the flame in a laboratory frame of reference U_f as a function of time, for several values of the exothermicity parameter K. Here, β = 10, Le = 1, ν_F = 1, and the initial time is defined by $\Psi(t = 0) = \Psi_0 = 10$

$$x_f = \Psi\left(1 + \frac{K\,\bar{H}\,\tanh(\Psi/Le\,b)}{(\Psi/Le\,b)}\right). \tag{144}$$

$$U_f = \frac{dx_f}{dt} = (1 + K\,\bar{H})\Psi' + \frac{K\,\bar{H}\,\tanh(\Psi/Le\,b)}{b}, \tag{145}$$

$$u_f = \frac{K\,\bar{H}\,\tanh(\Psi/Le\,b)}{b}; \tag{146}$$

$$N = \Psi\left[1 - \frac{\tanh(\Psi/d)}{(\Psi/d)}\right]. \tag{147}$$

Results are given in Figs. 9-11.

NONISOBARIC ASPECTS OF FLAME/WALL INTERACTION

For a contained premixture, the isobaric approximation requires reconsideration, and the initial/boundary-value problem, as presented in Eqs. 22, 34-47, is to be examined. The integral-equation approach, developed above for isobaric interaction of a flame with both a cold isothermal wall and also an adiabatic wall, has been generalized to the nonisobaric case for both types of wall boundary conditions. The generalization does require simultaneous solution of six quasilinear coupled ordinary differential equations, since the spatially invariant pressure, p(t), joins the five unknown functions treated for the isobaric case. Integration of the middle equation of Eq. 22 over the flow domain, enforcement of the impervious condition on the velocity at the containing walls, and substitution of the adopted spatial variation of the temperature yield the sixth equation to complement the five obtained from Eqs. 35-37, 40-41. Details and results are reserved for another publication.

The conjecture here is that significant flame/wall interaction occurs over a few diffusion scales only; thus, as long as the bulk-gas flame speed is appreciable (i.e., the premixture is not so fuel-lean that the laminar propagation speed is highly retarded), the quenching of the flame near a cold wall, or the acceleration of the flame near an adiabatic wall, is isobaric. The compression-enhanced pressure level attained by the burning of the entire confined mass of gas is the pressure level to use in the near-wall analyses. The final pressure attained in a homogeneous fuel-lean premixture, uniformly at pressure p_u^* at the initiation of burning in a container of length L^*, may be shown by thermodynamic arguments to be $p_f^* = p_u^* + (\gamma-1)\cdot Y_{Fu}\,\rho_u^*\,Q^*\,L^*$, in the absence of losses (which may be substantial). The anticipation is that results obtained from an integral-equation method for a confined premixture will confirm the conjecture that flame/wall interaction is virtually isobaric, as far as compression from confinement is concerned.

However, there may be significant pressure change over the time interval of flame/wall

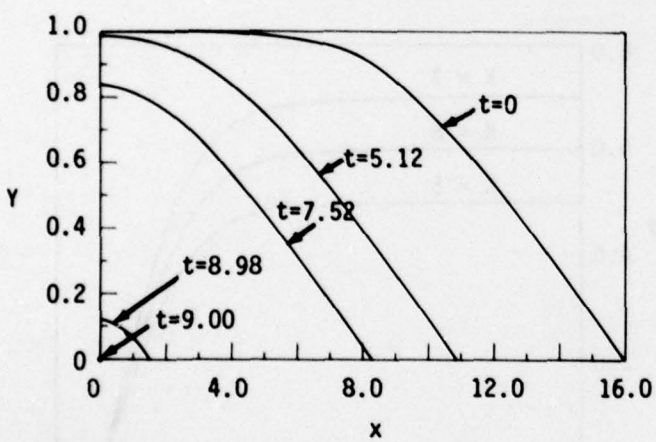

Fig. 9 - From integral-method results for an adiabatic wall, profiles of the (normalized, stoichiometrically adjusted) fuel mass fraction Y as a function of the dimensionless Cartesian coordinate x, at several times t, where the initial position of the flame in von Mises coordinates $\Psi_0 = 10$. For this nominal case, Le = 1, K = 6. Since the nondimensional temperature T = 1 - Y, the wall temperature T(0,t) rises rapidly to the adiabatic flame temperature

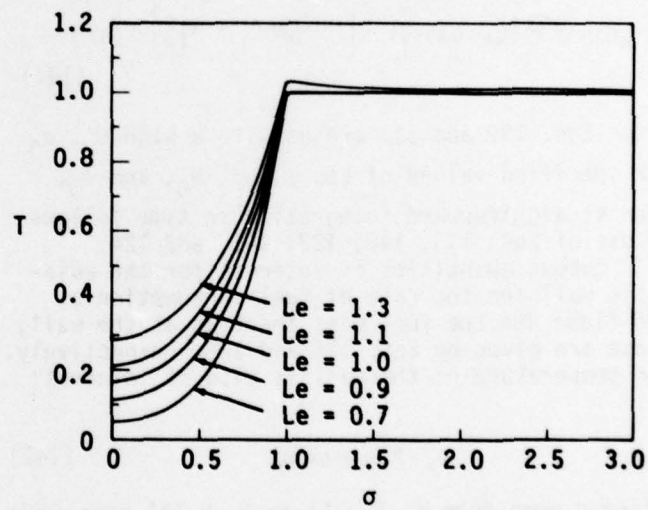

Fig. 10a - From integral-method results for an adiabatic wall, profiles of the dimensionless temperature T as a function of $\sigma(= \psi/\Psi$, where ψ is the von Mises spatial coordinate and Ψ is the flame position), at time t = 7.52, where $\Psi_0 = \Psi(t = 0) = 10$, for several values of the Lewis-Semenov number Le. Here the dimensionless Arrhenius activation temperature $\beta = 10$, the stoichiometric coefficient for fuel $\nu_F = 1$, the exothermicity factor K = 6. Augmenting the thermal diffusivity preheats the unburned fuel more effectively

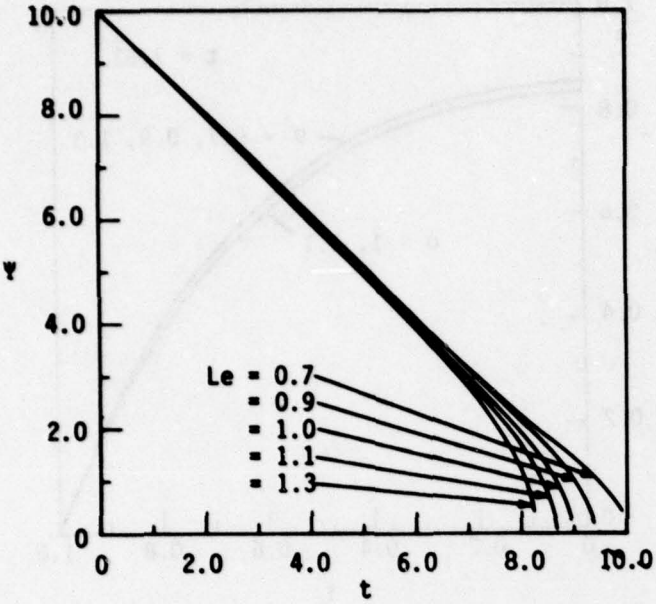

Fig. 10b - From integral-method results for an adiabatic wall, the flame position in von Mises coordinates Ψ as a function of time t, for several values of the Lewis-Semenov number Le. Here, $\beta = 10$, $\nu_F = 1$, $K = 6$. The larger the Lewis number, the more rapid the final acceleration (from an initially constant-speed propagation) of the thin flame into the wall, owing to interaction with the wall; because of large terminal gradients, the calculation is not completed except for Le = 1, though $\Psi \to 0$ at finite time in the model

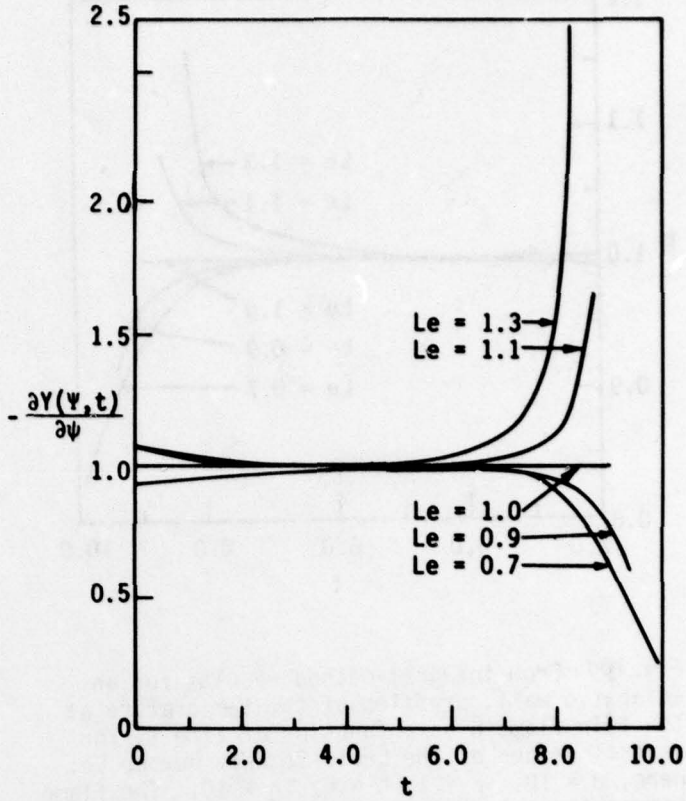

Fig. 10c - From integral-method results for an adiabatic wall, profiles of the dimensionless fuel consumption at the thin flame, $-\partial Y(\Psi,t)/\partial t$ as a function of time t, for several values of the Lewis-Semenov number Le. Here $\beta = 10$, $\nu_F = 1$, $K = 6$, $\Psi_0 = 10$. The consumption rate at a fixed time increases monotonically with Lewis number after flame-wall interaction begins

interaction from piston motion during operation at higher rates of revolution [14]. Prescribed movement of a wall in time presumably suffices to simulate piston motion in the one-dimensional unsteady reacting flows under study. It is worth emphasizing that it is piston motion (and, hence, wall motion) that is prescribed as a function of time; the wall motion must be translated into a variation of pressure with time.

DISCUSSION AND SUMMARY

The following properties of results, obtained by use of a thin-flame model to describe isobaric unsteady one-dimensional laminar flame propagation through a fuel-lean premixture under a direct one-step irreversible exothermic chemical reaction, seem worth noting.

First, for a spatially unbounded domain, the effect of heat extraction from, or of heat addition to, a flame, on the rate of recovery both of steady propagation and of flame temperature are recalled to be as follows. The rate of recovery is faster for larger Lewis-Semenov number, and for flame-temperature augmentation (as opposed to flame-temperature depression). For too large a flame-temperature depression, steady flame propagation is not recovered at all, at least not for that time span of practical interest for many purposes. These results are obtained here by approximate, integral-method treatment of a thin-flame formulation.

Second, also for a spatially unbounded domain, the transition between steady flame propagation at one stoichiometric ratio through a continuous change to steady flame propagation at an augmented (or decremented) stoichiometric ratio, is examined by means of numerical solution of simultaneous nonlinear Volterra integral equations, obtained by application of the Fourier transform to the thin-flame formulation (Figs. 2 through 4). The time required for transition through a given fuel stratification decreases with an increase in either the Lewis-Semenov

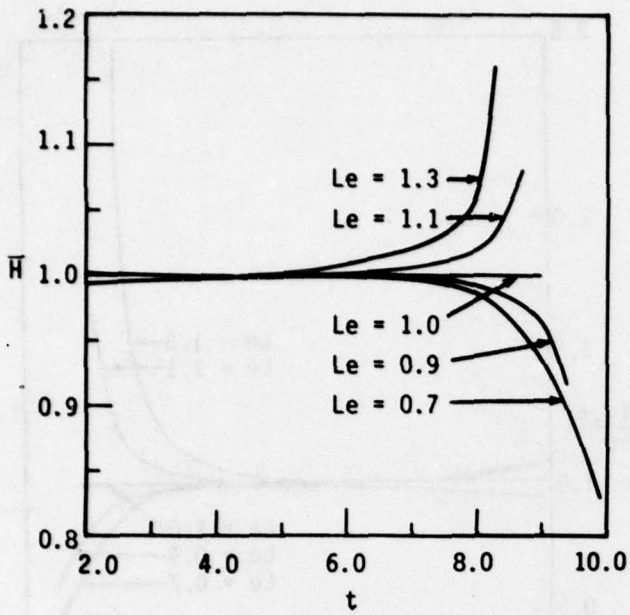

Fig. 10d - From integral-method results for an adiabatic wall, profiles of the temperature at the thin flame $\bar{H}$ as a function of time t, for several values of the Lewis-Semenov number Le. Here, $\beta = 10$, $\nu_F = 1$, $K = 6$, $\Psi_0 = 10$. The flame temperature at a fixed time increases monotonically with Lewis number after flame-wall interaction begins. Since $\bar{H}(t) = 1$ for Le = 1, the parameters ν_F, β play no role in this case

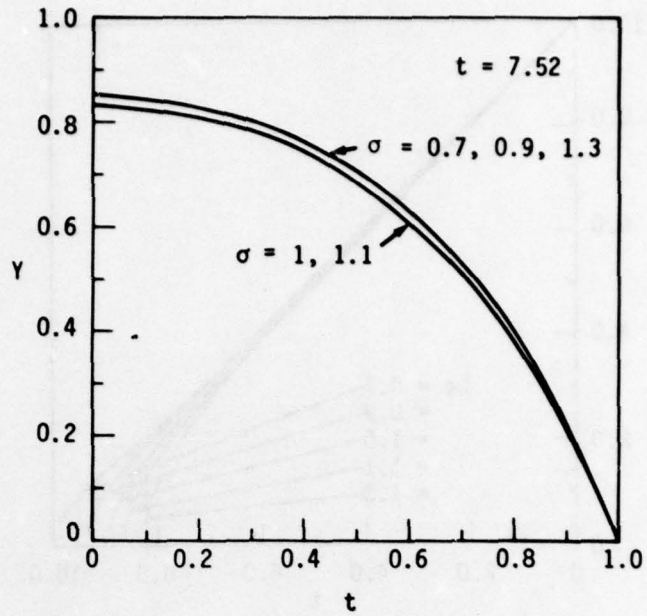

Fig. 11 - From integral-method results for an adiabatic wall, profiles of the (normalized, stoichiometrically adjusted) fuel mass fraction Y as a function of the coordinate $\sigma(= \psi/\Psi)$, at time t = 7.52, where $\Psi_0 = \Psi(t=0) = 10$, for several values of the Lewis-Semenov number Le. There is a slight depression of the value of Y for Le = 1; i.e., there is a nonmonotonic variation (according to the approximate method)

number, or the reaction order with respect to fuel, or the dimensionless Arrhenius activation energy, or the sharpness of the fuel stratification. Also, the time requires for transition is less for propagation through a fuel enrichment of a given magnitude, as opposed to propagation through a fuel decrement of the same magnitude. Further, judicious use of a steady-flame-propagation relation yields the flame speed through the stratification, with error on the order of a few percent; that is, a quasisteady approximation normally should suffice to describe the flame speed and flame temperature through the transition. Incidentally, with knowledge of the flame speed and flame temperature as a function of time, should the entire spatial profile for fuel and/or temperature be required, it seems numerically easier to return to the differential-equation formulation to obtain results, rather than to seek such information from the integral-equation formulation.

Third, attention is turned to results from integral-method treatment of the retardation of flame propagation as a cold wall is approached (Figs. 5-8). The cold-wall problem (and other problems) have already been treated by Buckmaster [31] by the thin-flame approximation. However, we are unable to infer from his paper the results in any of our figures 5a-5e, 6a-6c, 7, and 8, except that for the flame position Ψ at Lewis-Semenov number Le = 1 in Fig. 6a. We have included the details of our treatment because we believe the differences in methodology to be of interest. The results in our figures are more readily compared with solutions furnished by Kurkov and Mirsky [10] and by Adamczyk and Lavoie [14], who use numerical integration of the initial/boundary-value problem with a conventional law-of-mass-action expression for the chemical-reaction term. The position of the propagating flame Ψ appears to reach a position of closest approach to the wall and then to retreat; the reversal occurs further from the wall at larger values of the dimensionless Arrhenius activation energy β. Because the larger-activation-energy flame maintains a greater distance from the wall, the flame temperature $\bar{H}$ decreases less rapidly in time. Raising the reaction order with respect to fuel ν_F also leads to closer approach of the flame to the wall and, hence, to a more rapid decrease in flame temperature. Increasing the Lewis-Semenov number Le likewise leads to more rapid decrease of the flame temperature owing to greater heat

transfer to the cold wall. Two other properties of the results are: (1) the rate of reactant consumption at the thin flame, $-\partial Y(\Psi,t)/\partial t$, decreases monotonically in time as the cold wall is approached; and (2) the speed of the flame in laboratory coordinates U_f increases significantly with flame exothermicity K in the bulk gas, but as the wall is approached and chemical activity is reduced, the distinction in the flame speed owing variation in K is much less prominent.

Fourth, from integral-method treatment of flame propagation toward an adiabatic wall (Figs. 9-11), there is a terminal acceleration of the flame toward the wall, increasingly pronounced as the Lewis-Semenov number Le achieves values in excess of unity; the total amount of fuel is consumed in finite time. The preheating of remaining fuel is greater for larger Lewis-Semenov number, and the flame temperature can exceed the adiabatic flame temperature for $Le > 1$; for $Le < 1$, the flame temperature falls below the adiabatic flame temperature as the wall is approached. The wall temperature approaches the thin-flame temperature as the flame reaches the wall.

There are two questions concerning accuracy that arise in connection with the integral-method treatment of the thin-flame formulation of flame/wall interaction: first, how well does the approximate, integral-method solution satisfy the thin-flame iniitial/boundary-value problem; next, how well does the approximate, integral-method solution satisfy the initial/boundary-value problem with the law of mass action and the Arrhenius expression for the specific rate constant. The error is defined here as the absolute value of the residual obtained by substituting the integral-method solution into the initial/boundary-value problem, normalized by the absolute magnitude of the largest term. For the Landau (flame-stabilized) coordinate σ, there are three terms (temporal variation, convective transport, diffusive transport) for the thin-flame formulation; there is a fourth term (chemical reaction) for the law-of-mass-action formulation. An error may be defined at any spatial point in the flow domain $0 \leq \sigma \leq \infty$ at any time $t \geq 0$. (The accuracy of the integral-method flame/wall-interaction results may be checked also be means of the Volterra-integral-equation formulation, presented above both for a cold, isothermal wall and also for an adiabatic wall; this procedure for checking accuracy is not adopted here.)

The error characterizing how well the integral-method solution approximates the solution to the thin-flame formulation seems acceptably small. For the preponderance of the flow domain in space and time, the error is 5% or less. At long times for $\sigma = 0.9$, the error increases to about 20%, but this is a very localized, peak value. For most of the spatial and temporal domain, the error characterizing how well the integral-method solution approximates the solution to the formulation with the law of mass action is approximately the same as the error incurred for the thin-flame formulation; i.e., the error remains small because the reaction-rate term is small. However, for $\sigma = 0.8$, 0.9 at large times, the error can become quite large [i.e., O(40%)]; this is especially true for a cold wall, since the quenched flame tends to be spatially diffuse. Nevertheless, the error incurred is quite localized.

Worthwhile directions for related further theoretical and experimental work include isobaric, spatially two-dimensional flame/wall interaction, and nonisobaric effects on flame propagation through premixtures confined by variable-volume containers. The flame-without-structure model seems a tractable means of examining such aerothermachemical flows. The application of transform techniques for the solution of such thin-flame models appears to be an approach deserving consideration.

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